Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-

Other names: Butyric acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-
Geraniol butyrate
Geranyl butyrate
Geranyl butanoate
Geranyl n-butyrate
n-Butyric acid, geranyl ester

Inchi: InChI=1S/C14H24O2/c1-5-7-14(15)16-11-10-13(4)9-6-8-12(2)3/h8,10H,5-7,9,11H2,1-4H

InchiKey: ZSBOMYJPSRFZAL-JLHYYAGUSA-N

Formula: C14H24O

SMILES: CCCC(=O)OCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 208.34

CAS: 106-29-6

Physical Properties

Property code	Value	Unit	Source
gf	-23.58	kJ/mol	Joback Method
hf	-362.23	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.022		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1523.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1563.00		NIST Webbook

rinpol	1544.00	NIST Webbook
rinpol	1566.00	NIST Webbook
rinpol	1544.00	NIST Webbook
rinpol	1565.00	NIST Webbook
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rinpol	1556.00	NIST Webbook
rinpol	1562.00	NIST Webbook
rinpol	1564.00	NIST Webbook
rinpol	1544.00	NIST Webbook

ripol	1877.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1901.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1900.00		NIST Webbook
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ripol	1888.00		NIST Webbook
ripol	1877.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1906.00		NIST Webbook
tb	604.09	K	Joback Method
tc	789.66	K	Joback Method
tf	281.62	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.10	J/mol×K	758.73	Joback Method
cpg	527.13	J/mol×K	604.09	Joback Method
cpg	543.66	J/mol×K	635.02	Joback Method
cpg	559.39	J/mol×K	665.95	Joback Method
cpg	574.35	J/mol×K	696.87	Joback Method
cpg	588.58	J/mol×K	727.80	Joback Method
cpg	614.97	J/mol×K	789.66	Joback Method
hvapt	68.60	kJ/mol	450.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106296&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume