2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (Z)-

Other names: 2,6-Octadien-1-ol, 3,7-dimethyl-, propionate, (Z)-
Neryl propionate
cis-3,7-Dimethyl-2,6-octadien-1-ol, propionate
Propionic acid, 3,7-dimethyl-2,6-octadien-1-yl ester
Propionic acid, neryl ester
Neryl propanoate

Inchi: InChI=1S/C13H22O2/c1-5-13(14)15-10-9-12(4)8-6-7-11(2)3/h7,9H,5-6,8,10H2,1-4H3/b1

InchiKey: BYCHQEILESTMQU-XFXZXTDPSA-N

Formula: C13H22O2

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

Mol. weight [g/mol]: 210.31

CAS: 105-91-9

Physical Properties

Property code	Value	Unit	Source
gf	-32.00	kJ/mol	Joback Method
hf	-341.59	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.632		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1515.40		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1432.00		NIST Webbook
ripol	1764.00		NIST Webbook

ripol	1794.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1782.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
tb	581.21	K	Joback Method
tc	768.75	K	Joback Method
tf	270.35	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.11	J/mol×K	581.21	Joback Method
cpg	492.09	J/mol×K	612.47	Joback Method
cpg	507.29	J/mol×K	643.72	Joback Method
cpg	521.75	J/mol×K	674.98	Joback Method
cpg	535.49	J/mol×K	706.24	Joback Method
cpg	548.55	J/mol×K	737.49	Joback Method
cpg	560.96	J/mol×K	768.75	Joback Method

Sources

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=C105908&Units=SI

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

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
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