

Glutaric acid, but-3-en-2-yl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C14H24O4/c1-6-11(4)17-13(15)8-7-9-14(16)18-12(5)10(2)3/h6,10-12H,1,7-9H
InchiKey:	BXEPMNXRQIVLRR-UHFFFAOYSA-N
Formula:	C14H24O4
SMILES:	C=CC(C)OC(=O)CCCC(=O)OC(C)C(C)C
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-320.32	kJ/mol	Joback Method
hf	-712.30	kJ/mol	Joback Method
hfus	25.74	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.862		Crippen Method
mvol	218.700	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1559.00		NIST Webbook
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tb	667.66	K	Joback Method
tc	853.72	K	Joback Method
tf	345.10	K	Joback Method
vc	0.831	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.34	J/molxK	667.66	Joback Method
cpg	616.23	J/molxK	698.67	Joback Method
cpg	631.30	J/molxK	729.68	Joback Method
cpg	645.58	J/molxK	760.69	Joback Method
cpg	659.07	J/molxK	791.70	Joback Method
cpg	671.77	J/molxK	822.71	Joback Method
cpg	683.70	J/molxK	853.72	Joback Method
dvisc	0.0029477	Paxs	345.10	Joback Method

dvisc	0.0011484	Paxs	398.86	Joback Method
dvisc	0.0005597	Paxs	452.62	Joback Method
dvisc	0.0003178	Paxs	506.38	Joback Method
dvisc	0.0002011	Paxs	560.14	Joback Method
dvisc	0.0001379	Paxs	613.90	Joback Method
dvisc	0.0001005	Paxs	667.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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