Glutaric acid, di(but-3-en-2-yl) ester

Inchi: InChI=1S/C13H20O4/c1-5-10(3)16-12(14)8-7-9-13(15)17-11(4)6-2/h5-6,10-11H,1-2,7-9H
InchiKey: LMIRESYEZCWSNC-UHFFFAOYSA-N
Formula: C13H20O4
SMILES: C=CC(C)OC(=O)CCCC(=O)OC(C)C=C
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-238.46	kJ/mol	Joback Method
hf	-560.95	kJ/mol	Joback Method
hfus	25.39	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.392		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
tb	641.90	K	Joback Method
tc	829.29	K	Joback Method
tf	347.07	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.38	J/mol×K	641.90	Joback Method
cpg	589.97	J/mol×K	798.05	Joback Method
cpg	578.28	J/mol×K	766.82	Joback Method
cpg	565.89	J/mol×K	735.59	Joback Method
cpg	552.78	J/mol×K	704.36	Joback Method
cpg	538.95	J/mol×K	673.13	Joback Method
cpg	600.96	J/mol×K	829.29	Joback Method
dvisc	0.0001282	Pa×s	641.90	Joback Method

dvisc	0.0001706	Pa×s	592.76	Joback Method
dvisc	0.0002392	Pa×s	543.62	Joback Method
dvisc	0.0003588	Pa×s	494.49	Joback Method
dvisc	0.0005883	Pa×s	445.35	Joback Method
dvisc	0.0010905	Pa×s	396.21	Joback Method
dvisc	0.0024077	Pa×s	347.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405250&Units=SI
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

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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