Glutaric acid, hex-2-en-1-yl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C16H26O4/c1-4-5-6-7-12-19-15(17)9-8-10-16(18)20-13-11-14(2)3/h6-7,11H,4-

InchiKey: XUSBHGXYILGJPO-VOTSOKGWSA-N

Formula: C16H26O4

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

Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-232.11	kJ/mol	Joback Method
hf	-638.52	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1929.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	726.26	K	Joback Method
tc	913.61	K	Joback Method
tf	390.28	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.64	J/mol×K	726.26	Joback Method
cpg	702.33	J/mol×K	757.49	Joback Method
cpg	717.21	J/mol×K	788.71	Joback Method
cpg	731.29	J/mol×K	819.94	Joback Method
cpg	744.60	J/mol×K	851.16	Joback Method
cpg	757.18	J/mol×K	882.39	Joback Method
cpg	769.05	J/mol×K	913.61	Joback Method

Sources

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=U405329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume