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

Inchi: InChI=1S/C15H26O4/c1-11(2)9-10-18-14(16)7-6-8-15(17)19-13(5)12(3)4/h9,12-13H,6-8,

InchiKey: AXJNZKDGMIOKNO-UHFFFAOYSA-N

Formula: C15H26O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-325.63	kJ/mol	Joback Method
hf	-745.66	kJ/mol	Joback Method
hfus	32.03	kJ/mol	Joback Method
hvap	66.56	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.254		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1745.00		NIST Webbook
tb	698.34	K	Joback Method
tc	886.09	K	Joback Method
tf	354.09	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.32	J/mol×K	698.34	Joback Method
cpg	671.58	J/mol×K	729.63	Joback Method
cpg	686.99	J/mol×K	760.92	Joback Method
cpg	701.57	J/mol×K	792.22	Joback Method
cpg	715.33	J/mol×K	823.51	Joback Method
cpg	728.30	J/mol×K	854.80	Joback Method
cpg	740.48	J/mol×K	886.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393567&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
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