

Glutaric acid, 3-methylbut-2-en-1-yl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C16H28O4/c1-12(2)9-10-19-15(17)7-6-8-16(18)20-14(5)11-13(3)4/h9,13-14H,6
InchiKey:	HGXXKVKFNAFHIST-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	CC(C)=CCOC(=O)CCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-317.21	kJ/mol	Joback Method
hf	-766.30	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	68.78	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.644		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	721.22	K	Joback Method
tc	908.16	K	Joback Method
tf	365.36	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.06	J/mol×K	721.22	Joback Method
cpg	727.70	J/mol×K	752.38	Joback Method
cpg	743.46	J/mol×K	783.53	Joback Method
cpg	758.35	J/mol×K	814.69	Joback Method
cpg	772.39	J/mol×K	845.85	Joback Method
cpg	785.61	J/mol×K	877.00	Joback Method
cpg	798.02	J/mol×K	908.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392486&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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