

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

Inchi:	InChI=1S/C16H28O4/c1-5-14(6-2)12-20-16(18)9-7-8-15(17)19-11-10-13(3)4/h10,14H,5-9
InchiKey:	MGWICACRNOFRQC-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	CCC(CC)COC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-314.77	kJ/mol	Joback Method
hf	-761.02	kJ/mol	Joback Method
hfus	38.14	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.645		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	721.66	K	Joback Method
tc	906.27	K	Joback Method
tf	380.36	K	Joback Method
vc	0.955	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.57	J/mol×K	721.66	Joback Method
cpg	726.98	J/mol×K	752.43	Joback Method
cpg	742.54	J/mol×K	783.20	Joback Method
cpg	757.26	J/mol×K	813.96	Joback Method
cpg	771.17	J/mol×K	844.73	Joback Method
cpg	784.28	J/mol×K	875.50	Joback Method
cpg	796.60	J/mol×K	906.27	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=U391665&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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