

Glutaric acid, hexyl 3-methylbut-2-enyl ester

Inchi:	InChI=1S/C16H28O4/c1-4-5-6-7-12-19-15(17)9-8-10-16(18)20-13-11-14(2)3/h11H,4-10,1
InchiKey:	VRHNMFYREZUTCC-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	CCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-312.33	kJ/mol	Joback Method
hf	-755.74	kJ/mol	Joback Method
hfus	41.66	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.790		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2008.00		NIST Webbook
tb	722.10	K	Joback Method
tc	904.50	K	Joback Method
tf	395.36	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.07	J/mol×K	722.10	Joback Method
cpg	726.27	J/mol×K	752.50	Joback Method
cpg	741.64	J/mol×K	782.90	Joback Method
cpg	756.21	J/mol×K	813.30	Joback Method
cpg	769.98	J/mol×K	843.70	Joback Method
cpg	782.99	J/mol×K	874.10	Joback Method
cpg	795.23	J/mol×K	904.50	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=U360090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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