

Glutaric acid, phenethyl propyl ester

Inchi:	InChI=1S/C16H22O4/c1-2-12-19-15(17)9-6-10-16(18)20-13-11-14-7-4-3-5-8-14/h3-5,7-8
InchiKey:	GQILUCFUUHJKFB-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCCOC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-271.59	kJ/mol	Joback Method
hf	-626.64	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	71.80	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.896		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	744.74	K	Joback Method
tc	945.71	K	Joback Method
tf	440.82	K	Joback Method
vc	0.872	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.23	J/molxK	744.74	Joback Method
cpg	715.72	J/molxK	912.21	Joback Method
cpg	704.32	J/molxK	878.72	Joback Method
cpg	691.99	J/molxK	845.22	Joback Method
cpg	678.71	J/molxK	811.73	Joback Method
cpg	664.46	J/molxK	778.23	Joback Method
cpg	726.20	J/molxK	945.71	Joback Method
dvisc	0.0000931	Paxs	744.74	Joback Method

dvisc	0.0001200	Paxs	694.09	Joback Method
dvisc	0.0001609	Paxs	643.43	Joback Method
dvisc	0.0002269	Paxs	592.78	Joback Method
dvisc	0.0003411	Paxs	542.13	Joback Method
dvisc	0.0005579	Paxs	491.47	Joback Method
dvisc	0.0010214	Paxs	440.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358677&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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