

Glutaric acid, hexadecyl phenethyl ester

Inchi:	InChI=1S/C29H48O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-25-32-28(30)22-19-23-29(3
InchiKey:	CLKWOSVEGMJFIY-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-162.13	kJ/mol	Joback Method
hf	-894.96	kJ/mol	Joback Method
hfus	70.48	kJ/mol	Joback Method
hvap	100.74	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.967		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	780.69	kPa	Joback Method
rinpol	3486.00		NIST Webbook
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tb	1042.18	K	Joback Method
tc	1284.65	K	Joback Method
tf	587.33	K	Joback Method
vc	1.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.72	J/molxK	1042.18	Joback Method
cpg	1452.53	J/molxK	1082.59	Joback Method
cpg	1469.48	J/molxK	1123.00	Joback Method
cpg	1484.64	J/molxK	1163.41	Joback Method
cpg	1498.12	J/molxK	1203.83	Joback Method
cpg	1510.00	J/molxK	1244.24	Joback Method
cpg	1520.37	J/molxK	1284.65	Joback Method
dvisc	0.0002365	Paxs	587.33	Joback Method

dvisc	0.0001126	Paxs	663.14	Joback Method
dvisc	0.0000625	Paxs	738.95	Joback Method
dvisc	0.0000387	Paxs	814.75	Joback Method
dvisc	0.0000260	Paxs	890.56	Joback Method
dvisc	0.0000186	Paxs	966.37	Joback Method
dvisc	0.0000139	Paxs	1042.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358692&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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