

Glutaric acid, pentadecyl 1-phenylpropyl ester

Inchi:	InChI=1S/C29H48O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-19-25-32-28(30)23-20-24-29(31)
InchiKey:	WEFRIJVVRIMXKW-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-164.57	kJ/mol	Joback Method
hf	-900.24	kJ/mol	Joback Method
hfus	66.96	kJ/mol	Joback Method
hvap	100.35	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.486		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	784.19	kPa	Joback Method
rinpol	3325.00		NIST Webbook
rinpol	3325.00		NIST Webbook
tb	1041.74	K	Joback Method
tc	1282.47	K	Joback Method
tf	572.33	K	Joback Method
vc	1.593	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.95	J/molxK	1041.74	Joback Method
cpg	1452.55	J/molxK	1081.86	Joback Method
cpg	1469.30	J/molxK	1121.98	Joback Method
cpg	1484.27	J/molxK	1162.11	Joback Method
cpg	1497.56	J/molxK	1202.23	Joback Method
cpg	1509.25	J/molxK	1242.35	Joback Method
cpg	1519.45	J/molxK	1282.47	Joback Method
dvisc	0.0002620	Paxs	572.33	Joback Method

dvisc	0.0001167	Paxs	650.56	Joback Method
dvisc	0.0000618	Paxs	728.80	Joback Method
dvisc	0.0000371	Paxs	807.03	Joback Method
dvisc	0.0000243	Paxs	885.27	Joback Method
dvisc	0.0000171	Paxs	963.50	Joback Method
dvisc	0.0000127	Paxs	1041.74	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=U358961&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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