

Glutaric acid, 2-methoxybenzyl tetradecyl ester

Inchi:	InChI=1S/C27H44O5/c1-3-4-5-6-7-8-9-10-11-12-13-16-22-31-26(28)20-17-21-27(29)32-2
InchiKey:	KYWWLDYLZBTWRL-UHFFFAOYSA-N
Formula:	C27H44O5
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1OC
Mol. weight [g/mol]:	448.64

Physical Properties

Property code	Value	Unit	Source
gf	-293.60	kJ/mol	Joback Method
hf	-997.37	kJ/mol	Joback Method
hfus	66.10	kJ/mol	Joback Method
hvap	99.36	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	7.153		Crippen Method
mcvol	388.280	ml/mol	McGowan Method
pc	855.46	kPa	Joback Method
rinpola	3328.00		NIST Webbook
tb	1023.82	K	Joback Method
tc	1258.07	K	Joback Method
tf	599.54	K	Joback Method
vc	1.506	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.61	J/molxK	1023.82	Joback Method
cpg	1352.63	J/molxK	1062.86	Joback Method
cpg	1367.73	J/molxK	1101.90	Joback Method
cpg	1380.96	J/molxK	1140.94	Joback Method
cpg	1392.36	J/molxK	1179.99	Joback Method
cpg	1401.98	J/molxK	1219.03	Joback Method
cpg	1409.86	J/molxK	1258.07	Joback Method
dvisc	0.0001845	Paxs	599.54	Joback Method
dvisc	0.0000963	Paxs	670.25	Joback Method

dvisc	0.0000569	Paxs	740.97	Joback Method
dvisc	0.0000369	Paxs	811.68	Joback Method
dvisc	0.0000256	Paxs	882.39	Joback Method
dvisc	0.0000188	Paxs	953.11	Joback Method
dvisc	0.0000144	Paxs	1023.82	Joback Method

Sources

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=U376938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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