

Glutaric acid, monoamide, N-tetradecyl-, octyl ester

Inchi:	InChI=1S/C27H53NO3/c1-3-5-7-9-11-12-13-14-15-16-17-19-24-28-26(29)22-21-23-27(30)
InchiKey:	KMFJIKLGMKZLSU-UHFFFAOYSA-N
Formula:	C27H53NO3
SMILES:	CCCCCCCCCCCCCNC(=O)CCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	439.71

Physical Properties

Property code	Value	Unit	Source
gf	-96.99	kJ/mol	Joback Method
hf	-904.52	kJ/mol	Joback Method
hfus	75.17	kJ/mol	Joback Method
hvap	98.03	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	7.878		Crippen Method
mcvol	410.280	ml/mol	McGowan Method
pc	735.22	kPa	Joback Method
rinqol	3318.00		NIST Webbook
tb	997.49	K	Joback Method
tc	1237.18	K	Joback Method
tf	568.80	K	Joback Method
vc	1.613	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.26	J/molxK	997.49	Joback Method
cpg	1466.54	J/molxK	1037.44	Joback Method
cpg	1487.00	J/molxK	1077.39	Joback Method
cpg	1505.72	J/molxK	1117.34	Joback Method
cpg	1522.79	J/molxK	1157.29	Joback Method
cpg	1538.31	J/molxK	1197.23	Joback Method
cpg	1552.38	J/molxK	1237.18	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=U360801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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