

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

Inchi: InChI=1S/C28H55NO3/c1-3-5-7-9-11-12-13-14-15-16-18-20-25-29-27(30)23-22-24-28(31)
InchiKey: QMQGJRAYCRVAET-UHFFFAOYSA-N
Formula: C28H55NO3
SMILES: CCCCCCCCCCCCCCNC(=O)CCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 453.74

Physical Properties

Property code	Value	Unit	Source
gf	-88.57	kJ/mol	Joback Method
hf	-925.16	kJ/mol	Joback Method
hfus	77.76	kJ/mol	Joback Method
hvap	100.26	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.268		Crippen Method
mcvol	424.370	ml/mol	McGowan Method
pc	698.39	kPa	Joback Method
rinpol	3419.00		NIST Webbook
rinpol	3419.00		NIST Webbook
tb	1020.37	K	Joback Method
tc	1272.25	K	Joback Method
tf	580.07	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.28	J/mol×K	1020.37	Joback Method
cpg	1532.40	J/mol×K	1062.35	Joback Method
cpg	1553.49	J/mol×K	1104.33	Joback Method
cpg	1572.69	J/mol×K	1146.31	Joback Method
cpg	1590.10	J/mol×K	1188.29	Joback Method
cpg	1605.84	J/mol×K	1230.27	Joback Method
cpg	1620.02	J/mol×K	1272.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U360802&Units=SI

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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