Glutaric acid, monoamide, N-(2-octyl)-, undecyl ester

Inchi: InChI=1S/C24H47NO3/c1-4-6-8-10-11-12-13-14-16-21-28-24(27)20-17-19-23(26)25-22(3

InchiKey: OZYRASWDOMVIOM-UHFFFAOYSA-N

Formula: C24H47NO3

SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)NC(C)CCCCCC

Mol. weight [g/mol]: 397.63

Physical Properties

Property code	Value	Unit	Source
gf	-124.69	kJ/mol	Joback Method
hf	-847.88	kJ/mol	Joback Method
hfus	63.88	kJ/mol	Joback Method
hvap	90.97	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	6.706		Crippen Method
mcvol	368.010	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	3251.00		NIST Webbook
tb	928.41	K	Joback Method
tc	1138.72	K	Joback Method
tf	519.99	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.00	J/mol×K	928.41	Joback Method
cpg	1272.06	J/mol×K	963.46	Joback Method
cpg	1290.72	J/mol×K	998.51	Joback Method
cpg	1308.02	J/mol×K	1033.57	Joback Method
cpg	1324.01	J/mol×K	1068.62	Joback Method
cpg	1338.76	J/mol×K	1103.67	Joback Method
cpg	1352.32	J/mol×K	1138.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360859&Units=SI
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

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
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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