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

Inchi: InChI=1S/C25H49NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-21-26-24(27)19-16-20-25(28)2

InchiKey: HULXGHPUJZWFQU-UHFFFAOYSA-N

Formula: C25H49NO3

SMILES: CCCCCCCCCCCCCCNC(=O)CCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 411.66

Physical Properties

Property code	Value	Unit	Source
gf	-116.27	kJ/mol	Joback Method
hf	-868.52	kJ/mol	Joback Method
hfus	66.47	kJ/mol	Joback Method
hvap	93.19	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.953		Crippen Method
mcvol	382.100	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
rinpol	3086.00		NIST Webbook
tb	951.29	K	Joback Method
tc	1169.40	K	Joback Method
tf	531.26	K	Joback Method
vc	1.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.74	J/mol×K	951.29	Joback Method
cpg	1336.40	J/mol×K	987.64	Joback Method
cpg	1355.53	J/mol×K	1023.99	Joback Method
cpg	1373.20	J/mol×K	1060.34	Joback Method
cpg	1389.47	J/mol×K	1096.69	Joback Method
cpg	1404.41	J/mol×K	1133.04	Joback Method
cpg	1418.08	J/mol×K	1169.40	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=U360798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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