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

Inchi: InChI=1S/C23H45NO3/c1-4-5-6-7-8-9-10-11-12-13-19-24-22(25)17-14-18-23(26)27-20-1
InchiKey: KUOSBQGPXUHIEK-UHFFFAOYSA-N
Formula: C23H45NO3
SMILES: CCCCCCCCCCCCNC(=O)CCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 383.61

Physical Properties

Property code	Value	Unit	Source
gf	-133.11	kJ/mol	Joback Method
hf	-827.24	kJ/mol	Joback Method
hfus	61.29	kJ/mol	Joback Method
hvap	88.74	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.173		Crippen Method
mcvol	353.920	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
tb	905.53	K	Joback Method
tc	1109.16	K	Joback Method
tf	508.72	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.77	J/mol×K	905.53	Joback Method
cpg	1208.29	J/mol×K	939.47	Joback Method
cpg	1226.50	J/mol×K	973.41	Joback Method
cpg	1243.45	J/mol×K	1007.34	Joback Method
cpg	1259.18	J/mol×K	1041.28	Joback Method
cpg	1273.75	J/mol×K	1075.22	Joback Method
cpg	1287.19	J/mol×K	1109.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360870&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

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