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

Inchi: InChI=1S/C19H37NO3/c1-4-6-8-10-13-17(3)20-18(21)14-12-15-19(22)23-16-11-9-7-5-2/h
InchiKey: DOADKABPBYPGME-UHFFFAOYSA-N
Formula: C19H37NO3
SMILES: CCCCCCOC(=O)CCCC(=O)NC(C)CCCCCC
Mol. weight [g/mol]: 327.50

Physical Properties

Property code	Value	Unit	Source
gf	-166.79	kJ/mol	Joback Method
hf	-744.68	kJ/mol	Joback Method
hfus	50.93	kJ/mol	Joback Method
hvap	79.84	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.755		Crippen Method
mcvol	297.560	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	2754.00		NIST Webbook
tb	814.01	K	Joback Method
tc	1000.39	K	Joback Method
tf	463.64	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.07	J/mol×K	814.01	Joback Method
cpg	959.79	J/mol×K	845.07	Joback Method
cpg	976.50	J/mol×K	876.14	Joback Method
cpg	992.21	J/mol×K	907.20	Joback Method
cpg	1006.96	J/mol×K	938.26	Joback Method
cpg	1020.78	J/mol×K	969.33	Joback Method
cpg	1033.68	J/mol×K	1000.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360854&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