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

Inchi: InChI=1S/C22H43NO3/c1-4-6-8-10-11-12-14-19-26-22(25)18-15-17-21(24)23-20(3)16-13

InchiKey: BFKYAHGGWFBKEI-UHFFFAOYSA-N

Formula: C22H43NO3

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

Mol. weight [g/mol]: 369.58

Physical Properties

Property code	Value	Unit	Source
gf	-141.53	kJ/mol	Joback Method
hf	-806.60	kJ/mol	Joback Method
hfus	58.70	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.926		Crippen Method
mcvol	339.830	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	3064.00		NIST Webbook
tb	882.65	K	Joback Method
tc	1080.61	K	Joback Method
tf	497.45	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.11	J/mol×K	882.65	Joback Method
cpg	1145.13	J/mol×K	915.64	Joback Method
cpg	1162.92	J/mol×K	948.64	Joback Method
cpg	1179.54	J/mol×K	981.63	Joback Method
cpg	1195.02	J/mol×K	1014.62	Joback Method
cpg	1209.40	J/mol×K	1047.62	Joback Method
cpg	1222.71	J/mol×K	1080.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360857&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