Glutaric acid monoamide, N-(1,2,3,4-tetrahydronaphth-1-yl)-, isohexyl ester

Othernames: Glutaric acid, N-(1,2,3,4-tetrahydronaphth-1-yl)-, isohexyl ester
Inchi: InChI=1S/C21H31NO3/c1-16(2)8-7-15-25-21(24)14-6-13-20(23)22-19-12-5-10-17-9-3-4-
InchiKey: DGQLDOQQVXWQJM-UHFFFAOYSA-N
Formula: C21H31NO3
SMILES: CC(C)CCCOC(=O)CCCC(=O)NC1CCCc2ccccc21
Mol. weight [g/mol]: 345.48

Physical Properties

Property code	Value	Unit	Source
gf	1.48	kJ/mol	Joback Method
hf	-494.26	kJ/mol	Joback Method
hfus	45.79	kJ/mol	Joback Method
hvap	87.31	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.330		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2813.00		NIST Webbook
rinpol	2813.00		NIST Webbook
tb	902.44	K	Joback Method
tc	1118.15	K	Joback Method
tf	539.54	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.12	J/mol×K	902.44	Joback Method
cpg	971.45	J/mol×K	938.39	Joback Method
cpg	986.57	J/mol×K	974.34	Joback Method
cpg	1000.55	J/mol×K	1010.29	Joback Method
cpg	1013.45	J/mol×K	1046.25	Joback Method
cpg	1025.35	J/mol×K	1082.20	Joback Method
cpg	1036.32	J/mol×K	1118.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360207&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