Glutaric acid, monoamide, N-(1-phenylethyl)-, isohexyl ester

Inchi: InChI=1S/C19H29NO3/c1-15(2)9-8-14-23-19(22)13-7-12-18(21)20-16(3)17-10-5-4-6-11-
InchiKey: BWUJKMHGLBBFKA-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CC(C)CCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-56.82	kJ/mol	Joback Method
hf	-513.43	kJ/mol	Joback Method
hfus	41.45	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.013		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2478.00		NIST Webbook
tb	840.25	K	Joback Method
tc	1046.05	K	Joback Method
tf	475.06	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.73	J/mol×K	840.25	Joback Method
cpg	866.65	J/mol×K	874.55	Joback Method
cpg	881.44	J/mol×K	908.85	Joback Method
cpg	895.13	J/mol×K	943.15	Joback Method
cpg	907.78	J/mol×K	977.45	Joback Method
cpg	919.41	J/mol×K	1011.75	Joback Method
cpg	930.08	J/mol×K	1046.05	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360155&Units=SI

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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