Glutaric acid, monoamide, N-methyl-N-benzyl-, isohexyl ester

Inchi: InChI=1S/C19H29NO3/c1-16(2)9-8-14-23-19(22)13-7-12-18(21)20(3)15-17-10-5-4-6-11-
InchiKey: SEGGZZLPABMLLF-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CC(C)CCCOC(=O)CCCC(=O)N(C)Cc1ccccc1
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-32.99	kJ/mol	Joback Method
hf	-494.09	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.795		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2509.00		NIST Webbook
tb	802.96	K	Joback Method
tc	1002.69	K	Joback Method
tf	469.87	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.83	J/mol×K	802.96	Joback Method
cpg	849.46	J/mol×K	836.25	Joback Method
cpg	864.99	J/mol×K	869.54	Joback Method
cpg	879.47	J/mol×K	902.83	Joback Method
cpg	892.94	J/mol×K	936.11	Joback Method
cpg	905.45	J/mol×K	969.40	Joback Method
cpg	917.04	J/mol×K	1002.69	Joback Method

Sources

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=U360840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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