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

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

Physical Properties

Property code	Value	Unit	Source
gf	-30.55	kJ/mol	Joback Method
hf	-488.81	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.939		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2548.00		NIST Webbook
tb	803.40	K	Joback Method
tc	1001.00	K	Joback Method
tf	484.87	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.30	J/mol×K	803.40	Joback Method
cpg	848.76	J/mol×K	836.33	Joback Method
cpg	864.15	J/mol×K	869.27	Joback Method
cpg	878.52	J/mol×K	902.20	Joback Method
cpg	891.91	J/mol×K	935.13	Joback Method
cpg	904.37	J/mol×K	968.07	Joback Method
cpg	915.94	J/mol×K	1001.00	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=U360841&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

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