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

Inchi: InChI=1S/C17H25NO3/c1-14(2)13-21-17(20)11-7-10-16(19)18(3)12-15-8-5-4-6-9-15/h4-

InchiKey: PPJGPPYNXBYACX-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: CC(C)COC(=O)CCCC(=O)N(C)Cc1ccccc1

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-49.83	kJ/mol	Joback Method
hf	-452.81	kJ/mol	Joback Method
hfus	37.71	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.014		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	2298.00		NIST Webbook
tb	757.20	K	Joback Method
tc	958.71	K	Joback Method
tf	447.33	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.09	J/mol×K	757.20	Joback Method
cpg	734.30	J/mol×K	790.78	Joback Method
cpg	749.44	J/mol×K	824.37	Joback Method
cpg	763.57	J/mol×K	857.95	Joback Method
cpg	776.71	J/mol×K	891.54	Joback Method
cpg	788.92	J/mol×K	925.12	Joback Method
cpg	800.23	J/mol×K	958.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360837&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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