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

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

InchiKey: OYXHSBZAFSFMFR-UHFFFAOYSA-N

Formula: C17H25NO3

SMILES: CC(C)COC(=O)CCCC(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 291.39

Physical Properties

Property code	Value	Unit	Source
gf	-73.66	kJ/mol	Joback Method
hf	-472.15	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	77.27	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.233		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	2271.00		NIST Webbook
tb	794.49	K	Joback Method
tc	1001.84	K	Joback Method
tf	452.52	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.24	J/mol×K	794.49	Joback Method
cpg	750.79	J/mol×K	829.05	Joback Method
cpg	765.25	J/mol×K	863.61	Joback Method
cpg	778.65	J/mol×K	898.17	Joback Method
cpg	791.03	J/mol×K	932.73	Joback Method
cpg	802.43	J/mol×K	967.28	Joback Method
cpg	812.89	J/mol×K	1001.84	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=U360152&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