Glutaric acid, monoamide, N-(2-phenylpropyl)-, isobutyl ester

Inchi: InChI=1S/C18H27NO3/c1-14(2)13-22-18(21)11-7-10-17(20)19-12-15(3)16-8-5-4-6-9-16/h
InchiKey: HDJWBHJOCZKVBW-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CC(C)COC(=O)CCCC(=O)NCC(C)c1ccccc1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-65.24	kJ/mol	Joback Method
hf	-492.79	kJ/mol	Joback Method
hfus	38.86	kJ/mol	Joback Method
hvap	79.50	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.276		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2384.00		NIST Webbook
tb	817.37	K	Joback Method
tc	1023.63	K	Joback Method
tf	463.79	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.56	J/mol×K	817.37	Joback Method
cpg	808.30	J/mol×K	851.75	Joback Method
cpg	822.93	J/mol×K	886.12	Joback Method
cpg	836.49	J/mol×K	920.50	Joback Method
cpg	849.01	J/mol×K	954.88	Joback Method
cpg	860.54	J/mol×K	989.25	Joback Method
cpg	871.12	J/mol×K	1023.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360820&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