

Glutaric acid monoamide, N-(1,2,3,4-tetrahydronaphth-1-yl)-, isobutyl ester

Other names: Glutaric acid, N-(1,2,3,4-tetrahydronaphth-1-yl)-, isobutyl ester
Inchi: InChI=1S/C19H27NO3/c1-14(2)13-23-19(22)12-6-11-18(21)20-17-10-5-8-15-7-3-4-9-16(3)
InchiKey: NYRRXRMOJBZWR-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CC(C)COC(=O)CCCC(=O)NC1CCCCc2ccccc21
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
gf	-15.36	kJ/mol	Joback Method
hf	-452.98	kJ/mol	Joback Method
hfus	40.61	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.550		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	856.68	K	Joback Method
tc	1073.26	K	Joback Method
tf	517.00	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.41	J/mol×K	856.68	Joback Method
cpg	852.49	J/mol×K	892.78	Joback Method
cpg	867.38	J/mol×K	928.87	Joback Method
cpg	881.14	J/mol×K	964.97	Joback Method
cpg	893.84	J/mol×K	1001.07	Joback Method
cpg	905.53	J/mol×K	1037.17	Joback Method
cpg	916.29	J/mol×K	1073.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360204&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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