

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

Other names: Glutaric acid, N-(1,2,3,4-tetrahydronaphth-1-yl)-, butyl ester

Inchi: InChI=1S/C19H27NO3/c1-2-3-14-23-19(22)13-7-12-18(21)20-17-11-6-9-15-8-4-5-10-16(

InchiKey: GIVUYJMVHVYEOE-UHFFFAOYSA-N

Formula: C19H27NO3

SMILES: CCCOC(=O)CCCC(=O)NC1CCCC2CCCCC21

Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
gf	-12.92	kJ/mol	Joback Method
hf	-447.70	kJ/mol	Joback Method
hfus	44.14	kJ/mol	Joback Method
hvap	83.25	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.694		Crippen Method
mcvol	262.940	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	2657.00		NIST Webbook
tb	857.12	K	Joback Method
tc	1071.21	K	Joback Method
tf	532.00	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.89	J/mol×K	857.12	Joback Method
cpg	851.80	J/mol×K	892.80	Joback Method
cpg	866.57	J/mol×K	928.48	Joback Method
cpg	880.24	J/mol×K	964.17	Joback Method
cpg	892.88	J/mol×K	999.85	Joback Method
cpg	904.56	J/mol×K	1035.53	Joback Method
cpg	915.33	J/mol×K	1071.21	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=U360205&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
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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