

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

Other names:

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

Inchi:

InChI=1S/C17H23NO3/c1-2-21-17(20)12-6-11-16(19)18-15-10-5-8-13-7-3-4-9-14(13)15/

InchiKey:

JUTQGDNWXNUHLG-UHFFFAOYSA-N

Formula:

C17H23NO3

SMILES:

CCOC(=O)CCCC(=O)NC1CCc2ccccc21

Mol. weight [g/mol]:

289.37

Physical Properties

Property code	Value	Unit	Source
gf	-29.76	kJ/mol	Joback Method
hf	-406.42	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	78.80	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.914		Crippen Method
mvol	234.760	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	2463.00		NIST Webbook
tb	811.36	K	Joback Method
tc	1028.40	K	Joback Method
tf	509.46	K	Joback Method
vc	0.893	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.27	J/molxK	811.36	Joback Method
cpg	735.86	J/molxK	847.53	Joback Method
cpg	750.32	J/molxK	883.71	Joback Method
cpg	763.69	J/molxK	919.88	Joback Method
cpg	776.04	J/molxK	956.06	Joback Method
cpg	787.43	J/molxK	992.23	Joback Method
cpg	797.91	J/molxK	1028.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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