

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

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

Inchi: InChI=1S/C20H29NO3/c1-2-3-6-15-24-20(23)14-8-13-19(22)21-18-12-7-10-16-9-4-5-11-

InchiKey: VYWHDYPGONTCEX-UHFFFAOYSA-N

Formula: C20H29NO3

SMILES: CCCCCOC(=O)CCCC(=O)NC1CCCCc2ccccc21

Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
gf	-4.50	kJ/mol	Joback Method
hf	-468.34	kJ/mol	Joback Method
hfus	46.73	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.084		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2752.00		NIST Webbook
tb	880.00	K	Joback Method
tc	1093.63	K	Joback Method
tf	543.27	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.90	J/mol×K	880.00	Joback Method
cpg	910.97	J/mol×K	915.60	Joback Method
cpg	925.87	J/mol×K	951.21	Joback Method
cpg	939.68	J/mol×K	986.81	Joback Method
cpg	952.45	J/mol×K	1022.42	Joback Method
cpg	964.25	J/mol×K	1058.02	Joback Method
cpg	975.14	J/mol×K	1093.63	Joback Method

Sources

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=U360206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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