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

Other names: Glutaric acid, N-(1,2,3,4-tetrahydronaphth-1-yl)-, octyl ester
Inchi: InChI=1S/C23H35NO3/c1-2-3-4-5-6-9-18-27-23(26)17-11-16-22(25)24-21-15-10-13-19-1
InchiKey: NYBPNWOYMYPPIW-UHFFFAOYSA-N
Formula: C23H35NO3
SMILES: CCCCCCCCOC(=O)CCCC(=O)NC1CCCc2ccccc21
Mol. weight [g/mol]: 373.53

Physical Properties

Property code	Value	Unit	Source
gf	20.76	kJ/mol	Joback Method
hf	-530.26	kJ/mol	Joback Method
hfus	54.50	kJ/mol	Joback Method
hvap	92.15	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.254		Crippen Method
mcvol	319.300	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	3073.00		NIST Webbook
rinpol	3073.00		NIST Webbook
tb	948.64	K	Joback Method
tc	1165.49	K	Joback Method
tf	577.08	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.08	J/mol×K	948.64	Joback Method
cpg	1092.68	J/mol×K	984.78	Joback Method
cpg	1108.06	J/mol×K	1020.92	Joback Method
cpg	1122.29	J/mol×K	1057.06	Joback Method
cpg	1135.45	J/mol×K	1093.20	Joback Method
cpg	1147.62	J/mol×K	1129.34	Joback Method
cpg	1158.88	J/mol×K	1165.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360210&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

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