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

Other names: Glutaric acid, N-(1,2,3,4-tetrahydronaphth-1-yl)-, heptyl ester
Inchi: InChI=1S/C22H33NO3/c1-2-3-4-5-8-17-26-22(25)16-10-15-21(24)23-20-14-9-12-18-11-6
InchiKey: VGLJNHQTAMAFLU-UHFFFAOYSA-N
Formula: C22H33NO3
SMILES: CCCCCCCOC(=O)CCCC(=O)NC1CCCc2ccccc21
Mol. weight [g/mol]: 359.50

Physical Properties

Property code	Value	Unit	Source
gf	12.34	kJ/mol	Joback Method
hf	-509.62	kJ/mol	Joback Method
hfus	51.91	kJ/mol	Joback Method
hvap	89.93	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.864		Crippen Method
mcvol	305.210	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2974.00		NIST Webbook
tb	925.76	K	Joback Method
tc	1140.71	K	Joback Method
tf	565.81	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.05	J/mol×K	925.76	Joback Method
cpg	1031.45	J/mol×K	961.59	Joback Method
cpg	1046.65	J/mol×K	997.41	Joback Method
cpg	1060.73	J/mol×K	1033.24	Joback Method
cpg	1073.75	J/mol×K	1069.06	Joback Method
cpg	1085.79	J/mol×K	1104.89	Joback Method
cpg	1096.92	J/mol×K	1140.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360209&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