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

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

Inchi: InChI=1S/C21H31NO3/c1-2-3-4-7-16-25-21(24)15-9-14-20(23)22-19-13-8-11-17-10-5-6-

InchiKey: FXOCLNOECOSQTI-UHFFFAOYSA-N

Formula: C21H31NO3

SMILES: CCCCCCOC(=O)CCCC(=O)NC1CCCc2ccccc21

Mol. weight [g/mol]: 345.48

Physical Properties

Property code	Value	Unit	Source
hfus	49.32	kJ/mol	Joback Method
hvap	116.25	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.54		Cheméo Relay (1.0)
logp	4.474		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2855.00		NIST Webbook
rinpol	2855.00		NIST Webbook
tb	672.80	K	Cheméo Relay (1.0)
tf	354.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.64	J/mol×K	902.88	Joback Method
cpg	970.87	J/mol×K	938.53	Joback Method
cpg	985.92	J/mol×K	974.18	Joback Method
cpg	999.85	J/mol×K	1009.83	Joback Method
cpg	1012.75	J/mol×K	1045.48	Joback Method
cpg	1024.67	J/mol×K	1081.13	Joback Method
cpg	1035.67	J/mol×K	1116.78	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360208&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point