

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

Other names:

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

Inchi:

InChI=1S/C18H25NO3/c1-2-13-22-18(21)12-6-11-17(20)19-16-10-5-8-14-7-3-4-9-15(14)

InchiKey:

RAMPUCPUBCAYHC-UHFFFAOYSA-N

Formula:

C18H25NO3

SMILES:

CCCOC(=O)CCCC(=O)NC1CCCCc2ccccc21

Mol. weight [g/mol]:

303.40

Physical Properties

Property code	Value	Unit	Source
hfus	41.55	kJ/mol	Joback Method
logp	3.304		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2560.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.66	J/mol×K	834.24	Joback Method
cpg	793.42	J/mol×K	870.11	Joback Method
cpg	808.03	J/mol×K	905.99	Joback Method
cpg	821.57	J/mol×K	941.86	Joback Method
cpg	834.07	J/mol×K	977.74	Joback Method
cpg	845.61	J/mol×K	1013.61	Joback Method
cpg	856.24	J/mol×K	1049.49	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U360203&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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