1-Naphthyl N-propylcarbamate

Inchi: InChI=1S/C14H15NO2/c1-2-10-15-14(16)17-13-9-5-7-11-6-3-4-8-12(11)13/h3-9H,2,10H2
InchiKey: UXYGKIWSDXDEMU-UHFFFAOYSA-N
Formula: C14H15NO2
SMILES: CCCNC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 229.28

Physical Properties

Property code	Value	Unit	Source
hfus	30.57	kJ/mol	Joback Method
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-4.15		Cheméo Relay (1.0)
logp	3.338		Crippen Method
mcvol	182.320	ml/mol	McGowan Method
tb	608.92	K	Cheméo Relay (1.0)
tf	322.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.05	J/mol×K	696.82	Joback Method
cpg	499.08	J/mol×K	734.24	Joback Method
cpg	512.12	J/mol×K	771.67	Joback Method
cpg	524.23	J/mol×K	809.09	Joback Method
cpg	535.47	J/mol×K	846.52	Joback Method
cpg	545.89	J/mol×K	883.94	Joback Method
cpg	555.56	J/mol×K	921.37	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25216277&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point