

N-ethyl-5-methyl-2-propan-2-ylcyclohexane-1-carb

Inchi:	InChI=1S/C13H25NO/c1-5-14-13(15)12-8-10(4)6-7-11(12)9(2)3/h9-12H,5-8H2,1-4H3,(H,
InchiKey:	VUNOFAIHSALQQH-UHFFFAOYSA-N
Formula:	C13H25NO
SMILES:	CCNC(=O)C1CC(C)CCC1C(C)C
Mol. weight [g/mol]:	211.35
CAS:	39711-79-0

Physical Properties

Property code	Value	Unit	Source
hfus	26.58	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Cheméo Relay (1.0)
logp	2.831		Crippen Method
mcvol	194.720	ml/mol	McGowan Method
tb	538.17	K	Cheméo Relay (1.0)
tc	765.04	K	Cheméo Relay (1.0)
tf	361.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-5.81890e+01
Coeff. B	1.36208e+00
Coeff. C	-6.86700e-04
Coeff. D	9.76600e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
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
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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