

1-Naphthylurea

Inchi:	InChI=1S/C11H10N2O/c12-11(14)13-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H3,12,13,14)
InchiKey:	FVSUYFWWFUVGRG-UHFFFAOYSA-N
Formula:	C11H10N2O
SMILES:	NC(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]:	186.21
CAS:	6950-84-1

Physical Properties

Property code	Value	Unit	Source
hf	-89.14	kJ/mol	Cheméo Relay (1.0)
hfus	26.81	kJ/mol	Joback Method
hvap	90.68	kJ/mol	Cheméo Relay (1.0)
ie	7.99	eV	Cheméo Relay (1.0)
log10ws	-3.34		Cheméo Relay (1.0)
logp	2.330		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
tb	605.25	K	Cheméo Relay (1.0)
tf	492.65	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	-4.55200e+01
Coeff. B	1.01680e+00
Coeff. C	-7.48780e-04
Coeff. D	2.13860e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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

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