Cyclopropanecarboxamide, N-(1-naphthyl)-

Inchi: InChI=1S/C14H13NO/c16-14(11-8-9-11)15-13-7-3-5-10-4-1-2-6-12(10)13/h1-7,11H,8-9H
InchiKey: POMQVLRIIXEWDN-UHFFFAOYSA-N
Formula: C14H13NO
SMILES: O=C(Nc1cccc2ccccc12)C1CC1
Mol. weight [g/mol]: 211.26

Physical Properties

Property code	Value	Unit	Source
gf	297.65	kJ/mol	Joback Method
hf	97.53	kJ/mol	Joback Method
hfus	27.52	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.188		Crippen Method
mcvol	165.590	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	2066.00		NIST Webbook
tb	681.14	K	Joback Method
tc	924.21	K	Joback Method
tf	439.71	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.98	J/mol×K	681.14	Joback Method
cpg	458.65	J/mol×K	721.65	Joback Method
cpg	472.15	J/mol×K	762.16	Joback Method
cpg	484.62	J/mol×K	802.67	Joback Method
cpg	496.18	J/mol×K	843.18	Joback Method
cpg	506.97	J/mol×K	883.70	Joback Method
cpg	517.13	J/mol×K	924.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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