Cyclopentanecarboxamide, N-(1-naphthyl)-

Inchi: InChI=1S/C16H17NO/c18-16(13-7-1-2-8-13)17-15-11-5-9-12-6-3-4-10-14(12)15/h3-6,9-1
InchiKey: OIAFDYISGAVWKU-UHFFFAOYSA-N
Formula: C16H17NO
SMILES: O=C(Nc1cccc2ccccc12)C1CCCC1
Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
gf	290.29	kJ/mol	Joback Method
hf	43.93	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.969		Crippen Method
mcvol	193.770	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	2304.00		NIST Webbook
tb	735.44	K	Joback Method
tc	983.34	K	Joback Method
tf	455.21	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.95	J/mol×K	735.44	Joback Method
cpg	570.84	J/mol×K	776.76	Joback Method
cpg	586.36	J/mol×K	818.07	Joback Method
cpg	600.64	J/mol×K	859.39	Joback Method
cpg	613.80	J/mol×K	900.71	Joback Method
cpg	625.98	J/mol×K	942.02	Joback Method
cpg	637.29	J/mol×K	983.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307032&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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