

N-Naphth-1-yl-3-oxobutanamide

Other names:	Acetoacet «alpha»-naphthylamide Acetoacetamide, N-1-naphthyl- N-1-Naphthylacetoacetamide Acetamide, N-1-naphthylaceto- N-1-naphthyl-3-oxobutyramide
Inchi:	InChI=1S/C14H13NO2/c1-10(16)9-14(17)15-13-8-4-6-11-5-2-3-7-12(11)13/h2-8H,9H2,1H
InchiKey:	LKVXQCKDIYHFGZ-UHFFFAOYSA-N
Formula:	C14H13NO2
SMILES:	CC(=O)CC(=O)Nc1cccc2ccccc12
Mol. weight [g/mol]:	227.26

Physical Properties

Property code	Value	Unit	Source
af	0.6481		Cheméo Relay (1.0)
hfus	30.98	kJ/mol	Joback Method
ie	7.74	eV	Cheméo Relay (1.0)
log10ws	-2.92		Cheméo Relay (1.0)
logp	2.757		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	642.39	K	Cheméo Relay (1.0)
tc	939.32	K	Cheméo Relay (1.0)
tf	402.06	K	Cheméo Relay (1.0)
vc	0.627	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.12	J/mol×K	728.27	Joback Method
cpg	485.80	J/mol×K	767.14	Joback Method
cpg	497.50	J/mol×K	806.02	Joback Method
cpg	508.31	J/mol×K	844.89	Joback Method
cpg	518.31	J/mol×K	883.77	Joback Method
cpg	527.58	J/mol×K	922.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86839&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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