

Norbutylone, Ac

Inchi:	InChI=1S/C13H15NO4/c1-3-10(14-8(2)15)13(16)9-4-5-11-12(6-9)18-7-17-11/h4-6,10H,3
InchiKey:	QRLOIKIAMPXIP-UHFFFAOYSA-N
Formula:	C13H15NO4
SMILES:	CCC(NC(C)=O)C(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]:	249.26

Physical Properties

Property code	Value	Unit	Source
gf	-122.94	kJ/mol	Joback Method
hf	-445.89	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	1.513		Crippen Method
mcvol	184.270	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpola	2200.00		NIST Webbook
rinpola	2200.00		NIST Webbook
tb	756.26	K	Joback Method
tc	982.18	K	Joback Method
tf	500.57	K	Joback Method
vc	0.697	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.34	J/molxK	756.26	Joback Method
cpg	538.80	J/molxK	793.91	Joback Method
cpg	550.36	J/molxK	831.57	Joback Method
cpg	561.10	J/molxK	869.22	Joback Method
cpg	571.08	J/molxK	906.88	Joback Method
cpg	580.38	J/molxK	944.53	Joback Method
cpg	589.07	J/molxK	982.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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