

Buphedrone

Inchi:	InChI=1S/C11H15NO/c1-3-10(12-2)11(13)9-7-5-4-6-8-9/h4-8,10,12H,3H2,1-2H3
InchiKey:	DDPMGIMJSRUULN-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CCC(NC)C(=O)c1ccccc1
Mol. weight [g/mol]:	177.24
CAS:	408332-79-6

Physical Properties

Property code	Value	Unit	Source
gf	112.18	kJ/mol	Joback Method
hf	-98.23	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	1.867		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1427.60		NIST Webbook
rinpol	1427.60		NIST Webbook
tb	581.36	K	Joback Method
tc	797.40	K	Joback Method
tf	327.74	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.57	J/molxK	581.36	Joback Method
cpg	386.54	J/molxK	617.37	Joback Method
cpg	400.55	J/molxK	653.37	Joback Method
cpg	413.65	J/molxK	689.38	Joback Method
cpg	425.88	J/molxK	725.38	Joback Method
cpg	437.28	J/molxK	761.39	Joback Method
cpg	447.88	J/molxK	797.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C408332796&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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