

Neburon, HFBA

Inchi:	InChI=1S/C16H15Cl2F7N2O2/c1-3-4-7-26(2)13(29)27(9-5-6-10(17)11(18)8-9)12(28)14(1
InchiKey:	SIDAPOKJEUPPHI-UHFFFAOYSA-N
Formula:	C16H15Cl2F7N2O2
SMILES:	CCCCN(C)C(=O)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	471.20

Physical Properties

Property code	Value	Unit	Source
gf	-1238.30	kJ/mol	Joback Method
hf	-1680.58	kJ/mol	Joback Method
hfus	47.41	kJ/mol	Joback Method
hvap	71.55	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.011		Crippen Method
mcvol	272.510	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	794.80	K	Joback Method
tc	985.49	K	Joback Method
tf	557.57	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.04	J/mol×K	794.80	Joback Method
cpg	796.11	J/mol×K	826.58	Joback Method
cpg	806.37	J/mol×K	858.36	Joback Method
cpg	815.92	J/mol×K	890.14	Joback Method
cpg	824.85	J/mol×K	921.93	Joback Method
cpg	833.24	J/mol×K	953.71	Joback Method
cpg	841.20	J/mol×K	985.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220423&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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