Dichlofluanid

Other names: Methanesulfenamide, 1,1-dichloro-N-[(dimethylamino)sulfonyl]-1-fluoro-N-phenyl-
Sulfamide, N-[(dichlorofluoromethyl)thio]-N',N'-dimethyl-N-phenyl-
Bayer 47531
BAY 47531
Dichlofluanide
Elvaron
Eparen
Euparen
Oiparen
Pecudin
N'-Dichlorofluoromethylthio-NN-dimethyl-N'-phenylsulphamide
Aniline, N-((dichlorofluoromethyl)thio)-N-((dimethylamino)sulfonyl)-
Euparene
Ku 13-o32-c
KUE 13032c
N-(Dichlor-fluor-methyl-thio)-N',N'-dimethyl-N-phenyl-schwefel-saeurediamid
N-((Dichlorofluoromethyl)thio)-N',N'-dimethyl-N-phenylsulfamide
N,N-Dimethyl-N'-phenyl-N'-((fluorodichloromethyl)thio)sulfamide
1,1-Dichloro-N-((dimethylamino)sulfonyl)-1-fluoro-N-phenylmethanesulfenamide
Diclofluanide
NSC 218451

Inchi: InChI=1S/C9H11Cl2FN2O2S2/c1-13(2)18(15,16)14(17-9(10,11)12)8-6-4-3-5-7-8/h3-7H,1

InchiKey: WURGXGVFSMYFCG-UHFFFAOYSA-N

Formula: C9H11Cl2FN2O2S2

SMILES: CN(C)S(=O)(=O)N(SC(F)(Cl)Cl)c1ccccc1

Mol. weight [g/mol]: 333.23

CAS: 1085-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-292.38	kJ/mol	Joback Method
hf	-505.32	kJ/mol	Joback Method
hfus	38.72	kJ/mol	Joback Method
hvap	74.10	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.006		Crippen Method

mcvol	204.560	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	644.34	K	Joback Method
tc	868.70	K	Joback Method
tf	418.36	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.08	J/mol×K	644.34	Joback Method
cpg	493.20	J/mol×K	681.73	Joback Method
cpg	505.11	J/mol×K	719.13	Joback Method
cpg	515.86	J/mol×K	756.52	Joback Method
cpg	525.53	J/mol×K	793.91	Joback Method
cpg	534.16	J/mol×K	831.31	Joback Method
cpg	541.84	J/mol×K	868.70	Joback Method

Sources

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=C1085989&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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