

N,N'-[Methylenebis(2-chloro-4,1-phenylene)]bis(2,

Other names:

Propiorylamide,
N,N'-[methylenebis(2-chloro-4,1-phenylene)]bis[2,2,3,3,3-pentafluoro-
N,N'-[Methanediylbis(2-chlorobenzene-4,1-diyl)]bis(2,2,3,3,3-pentafluoropropionylamide)

Inchi:

InChI=1S/C19H10Cl2F10N2O2/c20-10-6-8(1-3-12(10)32-14(34)16(22,23)18(26,27)28)5-

InchiKey:

UNWQOSDILZWABJ-UHFFFAOYSA-N

Formula:

C19H10Cl2F10N2O2

SMILES:

O=C(Nc1ccc(Cc2ccc(NC(=O)C(F)(F)C(F)(F)F)c(Cl)c2)cc1Cl)C(F)(F)C(F)(F)F

Mol. weight [g/mol]:

559.18

Physical Properties

Property code	Value	Unit	Source
gf	-1744.26	kJ/mol	Joback Method
hf	-2154.11	kJ/mol	Joback Method
hfus	54.43	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	6.856		Crippen Method
mvol	296.330	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpol	2418.00		NIST Webbook
tb	970.12	K	Joback Method
tc	1189.46	K	Joback Method
tf	687.41	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.40	J/molxK	970.12	Joback Method
cpg	896.78	J/molxK	1006.68	Joback Method
cpg	904.75	J/molxK	1043.23	Joback Method
cpg	912.46	J/molxK	1079.79	Joback Method
cpg	920.08	J/molxK	1116.35	Joback Method
cpg	927.76	J/molxK	1152.91	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=U373483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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