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

Other names: Acetamide, N,N'-[methylenebis(2-chloro-4,1-phenylene)]bis[2,2,2-trifluoro-
N,N'-[Methanediylbis(2-chlorobenzene-4,1-diyl)]bis(2,2,2-trifluoroacetamide)
N-[2-Chloro-4-[[3-chloro-4-[(2,2,2-trifluoroacetyl)amino]phenyl]methyl]phenyl]-2,2,2-trifluo

Inchi: InChI=1S/C17H10Cl2F6N2O2/c18-10-6-8(1-3-12(10)26-14(28)16(20,21)22)5-9-2-4-13(1

InchiKey: XOAPUMLLYZSBIT-UHFFFAOYSA-N

Formula: C17H10Cl2F6N2O2

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

Mol. weight [g/mol]: 459.17

Physical Properties

Property code	Value	Unit	Source
gf	-987.54	kJ/mol	Joback Method
hf	-1310.89	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.586		Crippen Method
mcvol	261.070	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2453.00		NIST Webbook
tb	933.74	K	Joback Method
tc	1155.29	K	Joback Method
tf	657.67	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.44	J/mol×K	933.74	Joback Method
cpg	754.76	J/mol×K	970.66	Joback Method
cpg	762.40	J/mol×K	1007.59	Joback Method
cpg	769.48	J/mol×K	1044.51	Joback Method
cpg	776.10	J/mol×K	1081.44	Joback Method
cpg	782.36	J/mol×K	1118.36	Joback Method

cpg	788.36	J/mol×K	1155.29	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=U373067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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