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

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

Inchi: InChI=1S/C21H8Cl2F12N2O4/c22-10-6-8(1-3-12(10)36(14(38)18(24,25)26)15(39)19(27,

InchiKey: MBIFKDFNUVEJQS-UHFFFAOYSA-N

Formula: C21H8Cl2F12N2O4

SMILES: O=C(N(C(=O)C(F)(F)F)c1ccc(Cc2ccc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)c(Cl)c2)cc1Cl)C(

Mol. weight [g/mol]: 651.19

Physical Properties

Property code	Value	Unit	Source
gf	-2332.10	kJ/mol	Joback Method
hf	-2784.65	kJ/mol	Joback Method
hfus	64.81	kJ/mol	Joback Method
hvap	94.39	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	6.553		Crippen Method
mcvol	331.190	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2204.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1283.75	K	Joback Method
tf	770.61	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.12	J/mol×K	1046.70	Joback Method
cpg	1011.40	J/mol×K	1086.21	Joback Method
cpg	1019.60	J/mol×K	1125.72	Joback Method
cpg	1027.92	J/mol×K	1165.22	Joback Method
cpg	1036.61	J/mol×K	1204.73	Joback Method
cpg	1045.88	J/mol×K	1244.24	Joback Method

cpg	1055.95	J/mol×K	1283.75	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U373068&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
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