Acetamide, n-(1,1-bis(p-chlorophenyl)-2,2,2-trifluoroethyl)-

Inchi: InChI=1S/C16H12Cl2F3NO/c1-10(23)22-15(16(19,20)21,11-2-6-13(17)7-3-11)12-4-8-14(

InchiKey: NPRLBMKFRSLGSQ-UHFFFAOYSA-N

Formula: C16H12Cl2F3NO

SMILES: CC(=O)NC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(F)(F)F

Mol. weight [g/mol]: 362.17

CAS: 2247-71-4

Physical Properties

Property code	Value	Unit	Source
gf	-352.74	kJ/mol	Joback Method
hf	-619.87	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.935		Crippen Method
mcvol	230.120	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
tb	799.05	K	Joback Method
tc	1034.32	K	Joback Method
tf	517.00	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.72	J/mol×K	799.05	Joback Method
cpg	630.21	J/mol×K	838.26	Joback Method
cpg	640.68	J/mol×K	877.47	Joback Method
cpg	650.26	J/mol×K	916.68	Joback Method
cpg	659.08	J/mol×K	955.90	Joback Method
cpg	667.27	J/mol×K	995.11	Joback Method
cpg	674.96	J/mol×K	1034.32	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=C2247714&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume