Acetamide, n-(2,2,2-trifluoro-1,1-bis(p-fluorophenyl)ethyl)-

Inchi: InChI=1S/C16H12F5NO/c1-10(23)22-15(16(19,20)21,11-2-6-13(17)7-3-11)12-4-8-14(18)

InchiKey: LOOCAEGGZALYLF-UHFFFAOYSA-N

Formula: C16H12F5NO

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

Mol. weight [g/mol]: 329.26

CAS: 2247-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-718.50	kJ/mol	Joback Method
hf	-980.61	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.907		Crippen Method
mcvol	209.180	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
tb	722.73	K	Joback Method
tc	934.92	K	Joback Method
tf	458.34	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.18	J/mol×K	722.73	Joback Method
cpg	601.11	J/mol×K	758.09	Joback Method
cpg	612.97	J/mol×K	793.46	Joback Method
cpg	623.86	J/mol×K	828.82	Joback Method
cpg	633.87	J/mol×K	864.19	Joback Method
cpg	643.09	J/mol×K	899.55	Joback Method
cpg	651.63	J/mol×K	934.92	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=C2247781&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