2,2,2-Trifluoro-N-[4-[4-[(2,2,2-trifluoroacetyl)amino

Other names: N,N'-(Oxydi-4,1-phenylene)bis(2,2,2-trifluoroacetamide)
N,N'-(Oxydibenzene-4,1-diyl)bis(2,2,2-trifluoroacetamide)
Inchi: InChI=1S/C16H10F6N2O3/c17-15(18,19)13(25)23-9-1-5-11(6-2-9)27-12-7-3-10(4-8-12)2
InchiKey: ICELGZHOASOPJY-UHFFFAOYSA-N
Formula: C16H10F6N2O3
SMILES: O=C(Nc1ccc(Oc2ccc(NC(=O)C(F)(F)F)cc2)cc1)C(F)(F)F
Mol. weight [g/mol]: 392.25
CAS: 5252-79-9

Physical Properties

Property code	Value	Unit	Source
gf	-1057.84	kJ/mol	Joback Method
hf	-1368.05	kJ/mol	Joback Method
hfus	42.74	kJ/mol	Joback Method
hvap	78.37	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.481		Crippen Method
mcvol	228.370	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	848.46	K	Joback Method
tc	1059.98	K	Joback Method
tf	583.75	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.94	J/mol×K	848.46	Joback Method
cpg	691.53	J/mol×K	883.71	Joback Method
cpg	700.23	J/mol×K	918.97	Joback Method
cpg	708.13	J/mol×K	954.22	Joback Method
cpg	715.31	J/mol×K	989.47	Joback Method

cpg	721.85	J/mol×K	1024.73	Joback Method
cpg	727.84	J/mol×K	1059.98	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=C5252799&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

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