2,6-Diethylaniline, N,N-bis(pentafluoropropionyl)

Other names: 2-Bis(pentafluoropropionyl)amino-1,3-diethylbenzene
Inchi: InChI=1S/C16H13F10NO2/c1-3-8-6-5-7-9(4-2)10(8)27(11(28)13(17,18)15(21,22)23)12(2
InchiKey: UJELPYIOAIKGKM-UHFFFAOYSA-N
Formula: C16H13F10NO2
SMILES: CCc1cccc(CC)c1N(C(=O)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 441.26

Physical Properties

Property code	Value	Unit	Source
gf	-1906.81	kJ/mol	Joback Method
hf	-2313.71	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	56.99	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.066		Crippen Method
mcvol	243.360	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1257.00		NIST Webbook
tb	702.08	K	Joback Method
tc	874.53	K	Joback Method
tf	469.45	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.77	J/mol×K	702.08	Joback Method
cpg	732.83	J/mol×K	730.82	Joback Method
cpg	744.00	J/mol×K	759.56	Joback Method
cpg	754.36	J/mol×K	788.30	Joback Method
cpg	763.98	J/mol×K	817.04	Joback Method
cpg	772.95	J/mol×K	845.79	Joback Method
cpg	781.32	J/mol×K	874.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373196&Units=SI
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

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