

9,9-Bis(2-cyanoethyl)fluorene

Other names:	9,9-Fluorenedipropionitrile 9H-Fluorene-9,9-dipropionitrile Fluorene-9,9-bis(propionitrile) Fluorene-9,9-dipropionitrile Propionitrile, 3,3'-fluorene-9-ylidenedi- 9,9'-Fluorenedipropionitrile 9H-fluorene-9,9-dipropionitrile
Inchi:	InChI=1S/C19H16N2/c20-13-5-11-19(12-6-14-21)17-9-3-1-7-15(17)16-8-2-4-10-18(16)19
InchiKey:	COWHDUMHYFLLER-UHFFFAOYSA-N
Formula:	C19H16N2
SMILES:	N#CCCC1(CCC#N)c2cccc2-c2cccc21
Mol. weight [g/mol]:	272.34
CAS:	4425-97-2

Physical Properties

Property code	Value	Unit	Source
gf	660.48	kJ/mol	Joback Method
hf	444.75	kJ/mol	Joback Method
hfus	31.32	kJ/mol	Joback Method
hvap	83.14	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.561		Crippen Method
mvol	222.950	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
tb	900.04	K	Joback Method
tc	1147.79	K	Joback Method
tf	560.63	K	Joback Method
vc	0.906	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.65	J/mol×K	900.04	Joback Method
cpg	670.07	J/mol×K	941.33	Joback Method

cpg	685.98	J/mol×K	982.62	Joback Method
cpg	702.66	J/mol×K	1023.91	Joback Method
cpg	720.39	J/mol×K	1065.20	Joback Method
cpg	739.45	J/mol×K	1106.49	Joback Method
cpg	760.11	J/mol×K	1147.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4425972&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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