1,1,1,3,3,3-HEXAFLUORO-2,2-DI(3,4-XYLYL)PROP

Other names: 1,1'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[3,4-dimethylbenzene]
2,2-Bis-(3,4-dimethylphenyl)-hexafluoropropane
Benzene, 1,1'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[3,4-dimethyl-
Inchi: InChI=1S/C19H18F6/c1-11-5-7-15(9-13(11)3)17(18(20,21)22,19(23,24)25)16-8-6-12(2)1
InchiKey: GLFKFHJEFMLTOB-UHFFFAOYSA-N
Formula: C19H18F6
SMILES: Cc1ccc(C(c2ccc(C)c(C)c2)(C(F)(F)F)C(F)(F)F)cc1C
Mol. weight [g/mol]: 360.34

Physical Properties

Property code	Value	Unit	Source
af	0.5851		Cheméo Relay (1.0)
gf	-864.94	kJ/mol	Joback Method
hf	-1217.50	kJ/mol	Cheméo Relay (1.0)
hfus	27.73	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-6.98		Cheméo Relay (1.0)
logp	6.331		Crippen Method
mcvol	241.670	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
tb	570.61	K	Cheméo Relay (1.0)
tc	804.31	K	Cheméo Relay (1.0)
tf	340.94	K	Cheméo Relay (1.0)
vc	0.879	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.56	J/mol×K	693.33	Joback Method
cpg	701.54	J/mol×K	726.87	Joback Method
cpg	716.37	J/mol×K	760.42	Joback Method
cpg	730.15	J/mol×K	793.96	Joback Method
cpg	742.96	J/mol×K	827.50	Joback Method

cpg	754.90	J/mol×K	861.05	Joback Method
cpg	766.07	J/mol×K	894.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.00 ± 5.00	K	0.30	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65294204&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume