

3,3'-Bis(trifluoromethyl)diphenylmethane

Other names:	3,3'-Methylenebis(«alpha», «alpha», «alpha»-trifluorotoluene 3,3'-di(Trifluoromethyl)diphenylmethane di(3,3'-Trifluoromethylphenyl)methane Bis(3,3'-trifluoromethylphenyl)methane 3,3'-Methylenebis(alpha,alpha,alpha-trifluorotoluene
Inchi:	InChI=1S/C15H10F6/c16-14(17,18)12-5-1-3-10(8-12)7-11-4-2-6-13(9-11)15(19,20)21/h1
InchiKey:	GXGZHSTYPHZGGN-UHFFFAOYSA-N
Formula:	C15H10F6
SMILES:	FC(F)(F)c1cccc(Cc2cccc(C(F)(F)F)c2)c1
Mol. weight [g/mol]:	304.23
CAS:	86845-35-4

Physical Properties

Property code	Value	Unit	Source
gf	-882.20	kJ/mol	Joback Method
hf	-1096.97	kJ/mol	Joback Method
hfus	25.56	kJ/mol	Joback Method
hvap	47.37	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.315		Crippen Method
mcvol	185.310	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
tb	595.08	K	Joback Method
tc	794.72	K	Joback Method
tf	345.07	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.25	J/molxK	595.08	Joback Method
cpg	490.90	J/molxK	628.35	Joback Method
cpg	504.43	J/molxK	661.63	Joback Method
cpg	516.91	J/molxK	694.90	Joback Method

cpg	528.40	J/mol×K	728.18	Joback Method
cpg	539.00	J/mol×K	761.45	Joback Method
cpg	548.77	J/mol×K	794.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.00 ± 1.00	K	0.07	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86845354&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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