3,3'-METHYLENEBIS(ALPHA,ALPHA,ALPHA-TRIF

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

Physical Properties

Property code	Value	Unit	Source
hf	-1120.47	kJ/mol	Cheméo Relay (1.0)
hfus	25.56	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Cheméo Relay (1.0)
ie	9.27	eV	Cheméo Relay (1.0)
log10ws	-5.85		Cheméo Relay (1.0)
logp	5.315		Crippen Method
mcvol	185.310	ml/mol	McGowan Method
tb	548.84	K	Cheméo Relay (1.0)
tc	768.05	K	Cheméo Relay (1.0)
tf	358.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86845354&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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point