3-Trifluoromethyldiphenylmethane

Inchi: InChI=1S/C14H11F3/c15-14(16,17)13-8-4-7-12(10-13)9-11-5-2-1-3-6-11/h1-8,10H,9H2
InchiKey: SHNGXCGDFPNOCG-UHFFFAOYSA-N
Formula: C14H11F3
SMILES: FC(F)(F)c1cccc(Cc2ccccc2)c1
Mol. weight [g/mol]: 236.23
CAS: 75198-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-299.40	kJ/mol	Joback Method
hf	-467.78	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.296		Crippen Method
mcvol	165.910	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
tb	572.64	K	Joback Method
tc	792.45	K	Joback Method
tf	317.09	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.97	J/mol×K	572.64	Joback Method
cpg	415.83	J/mol×K	609.28	Joback Method
cpg	430.47	J/mol×K	645.91	Joback Method
cpg	443.94	J/mol×K	682.55	Joback Method
cpg	456.34	J/mol×K	719.18	Joback Method
cpg	467.75	J/mol×K	755.82	Joback Method
cpg	478.24	J/mol×K	792.45	Joback Method

Sources

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=C75198322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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