m-Trifluoromethoxybenzyl alcohol

Other names: 3-(Trifluoromethoxy) benzyl alcohol
Inchi: InChI=1S/C8H7F3O2/c9-8(10,11)13-7-3-1-2-6(4-7)5-12/h1-4,12H,5H2
InchiKey: XRGSSROOYSFMMS-UHFFFAOYSA-N
Formula: C8H7F3O2
SMILES: OCc1cccc(OC(F)(F)F)c1
Mol. weight [g/mol]: 192.14
CAS: 50823-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-704.15	kJ/mol	Joback Method
hf	-864.92	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.077		Crippen Method
mcvol	116.870	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
tb	523.28	K	Joback Method
tc	704.09	K	Joback Method
tf	306.10	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.04	J/mol×K	523.28	Joback Method
cpg	283.48	J/mol×K	553.41	Joback Method
cpg	292.38	J/mol×K	583.55	Joback Method
cpg	300.74	J/mol×K	613.68	Joback Method
cpg	308.60	J/mol×K	643.82	Joback Method
cpg	315.97	J/mol×K	673.95	Joback Method
cpg	322.88	J/mol×K	704.09	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=C50823900&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