Methyl 3-trifluoromethylbenzoate

Other names: Benzoic acid, 3-(trifluoromethyl)-, methyl ester
4-CF3-C6H4-COOCH3
Inchi: InChI=1S/C9H7F3O2/c1-14-8(13)6-3-2-4-7(5-6)9(10,11)12/h2-5H,1H3
InchiKey: QQHNNQCWKYFNAC-UHFFFAOYSA-N
Formula: C9H7F3O2
SMILES: COC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 204.15
CAS: 2557-13-3

Physical Properties

Property code	Value	Unit	Source
affp	826.60	kJ/mol	NIST Webbook
basg	795.70	kJ/mol	NIST Webbook
ea	0.60 ± 0.09	eV	NIST Webbook
ea	0.62 ± 0.09	eV	NIST Webbook
gf	-687.83	kJ/mol	Joback Method
hf	-845.91	kJ/mol	Joback Method
hfus	17.33	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.492		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	507.85	K	Joback Method
tc	706.00	K	Joback Method
tf	306.48	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.63	J/mol×K	507.85	Joback Method
cpg	295.99	J/mol×K	540.87	Joback Method
cpg	306.64	J/mol×K	573.90	Joback Method

cpg	316.61	J/mol×K	606.92	Joback Method
cpg	325.92	J/mol×K	639.95	Joback Method
cpg	334.60	J/mol×K	672.97	Joback Method
cpg	342.69	J/mol×K	706.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2557133&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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

Latest version available from:
https://www.chemeo.com/cid/15-360-5/Methyl-3-trifluoromethylbenzoate.pdf
Generated by Cheméo on 2024-04-28 23:42:27.57299483 +0000 UTC m=+16636996.493572146.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.