

Ethyl-3-trifluoromethyl benzoate

Other names:	Ethyl m-trifluoromethylbenzoate 3-Trifluoromethylbenzoic acid, ethyl ester
Inchi:	InChI=1S/C10H9F3O2/c1-2-15-9(14)7-4-3-5-8(6-7)10(11,12)13/h3-6H,2H2,1H3
InchiKey:	MHNBTKIAHHECCQ-UHFFFAOYSA-N
Formula:	C10H9F3O2
SMILES:	CCOC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	218.17
CAS:	76783-59-0

Physical Properties

Property code	Value	Unit	Source
gf	-679.41	kJ/mol	Joback Method
hf	-866.55	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
h vap	46.20	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.882		Crippen Method
m cvol	140.750	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
tb	530.73	K	Joback Method
tc	726.25	K	Joback Method
tf	317.75	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.54	J/molxK	530.73	Joback Method
cpg	340.77	J/molxK	563.32	Joback Method
cpg	352.26	J/molxK	595.90	Joback Method
cpg	363.03	J/molxK	628.49	Joback Method
cpg	373.10	J/molxK	661.08	Joback Method
cpg	382.52	J/molxK	693.66	Joback Method
cpg	391.31	J/molxK	726.25	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=C76783590&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

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