2,5-Di(trifluoromethyl)benzoic acid, ethyl ester

Inchi: InChI=1S/C11H8F6O2/c1-2-19-9(18)7-5-6(10(12,13)14)3-4-8(7)11(15,16)17/h3-5H,2H2,1
InchiKey: CXPOENCKRJUREO-UHFFFAOYSA-N
Formula: C11H8F6O2
SMILES: CCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 286.17

Physical Properties

Property code	Value	Unit	Source
gf	-1262.21	kJ/mol	Joback Method
hf	-1495.74	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	45.34	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.901		Crippen Method
mcvol	160.150	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1115.00		NIST Webbook
tb	553.17	K	Joback Method
tc	732.00	K	Joback Method
tf	345.73	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.10	J/mol×K	553.17	Joback Method
cpg	413.83	J/mol×K	582.97	Joback Method
cpg	424.82	J/mol×K	612.78	Joback Method
cpg	435.10	J/mol×K	642.58	Joback Method
cpg	444.71	J/mol×K	672.39	Joback Method
cpg	453.67	J/mol×K	702.19	Joback Method
cpg	462.01	J/mol×K	732.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338933&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume