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

Inchi: InChI=1S/C13H12F6O2/c1-2-3-6-21-11(20)9-7-8(12(14,15)16)4-5-10(9)13(17,18)19/h4-5
InchiKey: NDKMOGBAVSCBBB-UHFFFAOYSA-N
Formula: C13H12F6O2
SMILES: CCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 314.22

Physical Properties

Property code	Value	Unit	Source
gf	-1245.37	kJ/mol	Joback Method
hf	-1537.02	kJ/mol	Joback Method
hfus	29.13	kJ/mol	Joback Method
hvap	49.79	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.681		Crippen Method
mcvol	188.330	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
tb	598.93	K	Joback Method
tc	774.85	K	Joback Method
tf	368.27	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.87	J/mol×K	598.93	Joback Method
cpg	510.76	J/mol×K	628.25	Joback Method
cpg	522.86	J/mol×K	657.57	Joback Method
cpg	534.22	J/mol×K	686.89	Joback Method
cpg	544.86	J/mol×K	716.21	Joback Method
cpg	554.84	J/mol×K	745.53	Joback Method
cpg	564.17	J/mol×K	774.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338936&Units=SI

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