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

Inchi: InChI=1S/C13H12F6O3/c1-2-21-5-6-22-11(20)9-7-8(12(14,15)16)3-4-10(9)13(17,18)19/h
InchiKey: KNFYHNWUWXVCPA-UHFFFAOYSA-N
Formula: C13H12F6O3
SMILES: CCOCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 330.22

Physical Properties

Property code	Value	Unit	Source
gf	-1350.37	kJ/mol	Joback Method
hf	-1669.24	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	52.20	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.917		Crippen Method
mcvol	194.200	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1370.00		NIST Webbook
tb	621.35	K	Joback Method
tc	796.90	K	Joback Method
tf	390.50	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.73	J/mol×K	621.35	Joback Method
cpg	536.33	J/mol×K	650.61	Joback Method
cpg	548.18	J/mol×K	679.87	Joback Method
cpg	559.31	J/mol×K	709.12	Joback Method
cpg	569.75	J/mol×K	738.38	Joback Method
cpg	579.53	J/mol×K	767.64	Joback Method
cpg	588.68	J/mol×K	796.90	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=U357364&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume