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

Inchi: InChI=1S/C17H20F6O2/c1-3-5-6-11(4-2)10-25-15(24)13-9-12(16(18,19)20)7-8-14(13)17

InchiKey: SHOZCBZKTNDEAX-UHFFFAOYSA-N

Formula: C17H20F6O2

SMILES: CCCCC(CC)COC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 370.33

Physical Properties

Property code	Value	Unit	Source
gf	-1214.13	kJ/mol	Joback Method
hf	-1624.86	kJ/mol	Joback Method
hfus	35.96	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.097		Crippen Method
mcvol	244.690	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	1575.00		NIST Webbook
tb	690.01	K	Joback Method
tc	865.87	K	Joback Method
tf	398.35	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.70	J/mol×K	690.01	Joback Method
cpg	721.52	J/mol×K	719.32	Joback Method
cpg	735.46	J/mol×K	748.63	Joback Method
cpg	748.57	J/mol×K	777.94	Joback Method
cpg	760.88	J/mol×K	807.25	Joback Method
cpg	772.45	J/mol×K	836.56	Joback Method
cpg	783.31	J/mol×K	865.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357742&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