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

Inchi: InChI=1S/C15H16F6O2/c1-2-3-4-5-8-23-13(22)11-9-10(14(16,17)18)6-7-12(11)15(19,20)
InchiKey: MJGZUTPPEGZCSK-UHFFFAOYSA-N
Formula: C15H16F6O2
SMILES: CCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 342.28

Physical Properties

Property code	Value	Unit	Source
gf	-1228.53	kJ/mol	Joback Method
hf	-1578.30	kJ/mol	Joback Method
hfus	34.31	kJ/mol	Joback Method
hvap	54.25	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.461		Crippen Method
mcvol	216.510	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
tb	644.69	K	Joback Method
tc	818.80	K	Joback Method
tf	390.81	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.47	J/mol×K	644.69	Joback Method
cpg	613.28	J/mol×K	673.71	Joback Method
cpg	626.28	J/mol×K	702.73	Joback Method
cpg	638.51	J/mol×K	731.74	Joback Method
cpg	650.00	J/mol×K	760.76	Joback Method
cpg	660.78	J/mol×K	789.78	Joback Method
cpg	670.91	J/mol×K	818.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338939&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

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

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