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

Inchi: InChI=1S/C15H16F6O2/c1-9(2)4-3-7-23-13(22)11-8-10(14(16,17)18)5-6-12(11)15(19,20)

InchiKey: HPPDABQLSVHGCZ-UHFFFAOYSA-N

Formula: C15H16F6O2

SMILES: CC(C)CCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 342.28

Physical Properties

Property code	Value	Unit	Source
gf	-1230.97	kJ/mol	Joback Method
hf	-1583.58	kJ/mol	Joback Method
hfus	30.79	kJ/mol	Joback Method
hvap	53.86	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.317		Crippen Method
mcvol	216.510	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
tb	644.25	K	Joback Method
tc	820.91	K	Joback Method
tf	375.81	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.92	J/mol×K	644.25	Joback Method
cpg	613.98	J/mol×K	673.69	Joback Method
cpg	627.19	J/mol×K	703.14	Joback Method
cpg	639.59	J/mol×K	732.58	Joback Method
cpg	651.23	J/mol×K	762.02	Joback Method
cpg	662.14	J/mol×K	791.47	Joback Method
cpg	672.36	J/mol×K	820.91	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=U338938&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