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

Inchi: InChI=1S/C14H14F6O2/c1-2-3-4-7-22-12(21)10-8-9(13(15,16)17)5-6-11(10)14(18,19)20/

InchiKey: WGXUBPDVMRWRAC-UHFFFAOYSA-N

Formula: C14H14F6O2

SMILES: CCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 328.25

Physical Properties

Property code	Value	Unit	Source
gf	-1236.95	kJ/mol	Joback Method
hf	-1557.66	kJ/mol	Joback Method
hfus	31.72	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.071		Crippen Method
mcvol	202.420	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
tb	621.81	K	Joback Method
tc	796.67	K	Joback Method
tf	379.54	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.98	J/mol×K	621.81	Joback Method
cpg	561.36	J/mol×K	650.95	Joback Method
cpg	573.93	J/mol×K	680.10	Joback Method
cpg	585.74	J/mol×K	709.24	Joback Method
cpg	596.83	J/mol×K	738.38	Joback Method
cpg	607.23	J/mol×K	767.52	Joback Method
cpg	616.98	J/mol×K	796.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338937&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