2,5-Di(trifluoromethyl)benzoic acid, 6-chlorohexyl ester

Inchi: InChI=1S/C15H15ClF6O2/c16-7-3-1-2-4-8-24-13(23)11-9-10(14(17,18)19)5-6-12(11)15(2

InchiKey: ORIJBJXIHCZILS-UHFFFAOYSA-N

Formula: C15H15ClF6O2

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

Mol. weight [g/mol]: 376.72

Physical Properties

Property code	Value	Unit	Source
gf	-1240.46	kJ/mol	Joback Method
hf	-1594.04	kJ/mol	Joback Method
hfus	38.50	kJ/mol	Joback Method
hvap	58.63	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.680		Crippen Method
mcvol	228.750	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	1762.00		NIST Webbook
tb	682.12	K	Joback Method
tc	860.85	K	Joback Method
tf	420.73	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.01	J/mol×K	682.12	Joback Method
cpg	640.86	J/mol×K	711.91	Joback Method
cpg	652.90	J/mol×K	741.70	Joback Method
cpg	664.18	J/mol×K	771.49	Joback Method
cpg	674.73	J/mol×K	801.28	Joback Method
cpg	684.60	J/mol×K	831.06	Joback Method
cpg	693.83	J/mol×K	860.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357368&Units=SI

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