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

Inchi: InChI=1S/C15H14F6O2/c16-14(17,18)9-6-7-12(15(19,20)21)11(8-9)13(22)23-10-4-2-1-3-

InchiKey: UQTDQXGUPGUFQM-UHFFFAOYSA-N

Formula: C15H14F6O2

SMILES: O=C(OC1CCCCC1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 340.26

Physical Properties

Property code	Value	Unit	Source
gf	-1204.08	kJ/mol	Joback Method
hf	-1523.98	kJ/mol	Joback Method
hfus	26.14	kJ/mol	Joback Method
hvap	54.67	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.214		Crippen Method
mcvol	205.650	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	664.24	K	Joback Method
tc	863.45	K	Joback Method
tf	398.19	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.43	J/mol×K	664.24	Joback Method
cpg	607.37	J/mol×K	697.44	Joback Method
cpg	622.16	J/mol×K	730.64	Joback Method
cpg	635.84	J/mol×K	763.85	Joback Method
cpg	648.48	J/mol×K	797.05	Joback Method
cpg	660.14	J/mol×K	830.25	Joback Method
cpg	670.87	J/mol×K	863.45	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=U357740&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