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

Inchi: InChI=1S/C16H16F6O2/c17-15(18,19)11-6-7-13(16(20,21)22)12(8-11)14(23)24-9-10-4-2

InchiKey: XMTSLUJPILXFKS-UHFFFAOYSA-N

Formula: C16H16F6O2

SMILES: O=C(OCC1CCCCC1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 354.29

Physical Properties

Property code	Value	Unit	Source
gf	-1195.66	kJ/mol	Joback Method
hf	-1544.62	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	56.90	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.461		Crippen Method
mcvol	219.740	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1614.00		NIST Webbook
tb	687.12	K	Joback Method
tc	884.14	K	Joback Method
tf	409.46	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.08	J/mol×K	687.12	Joback Method
cpg	661.25	J/mol×K	719.96	Joback Method
cpg	676.26	J/mol×K	752.79	Joback Method
cpg	690.17	J/mol×K	785.63	Joback Method
cpg	703.04	J/mol×K	818.46	Joback Method
cpg	714.93	J/mol×K	851.30	Joback Method
cpg	725.90	J/mol×K	884.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357743&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