3-Trifluoromethylbenzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C16H20ClF3O2/c17-10-5-3-1-2-4-6-11-22-15(21)13-8-7-9-14(12-13)16(18,19)2

InchiKey: MRTHRZOLWFXNPF-UHFFFAOYSA-N

Formula: C16H20ClF3O2

SMILES: O=C(OCCCCCCCCCCl)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 336.78

Physical Properties

Property code	Value	Unit	Source
gf	-640.82	kJ/mol	Joback Method
hf	-1006.13	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	63.94	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.442		Crippen Method
mcvol	237.530	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	705.44	K	Joback Method
tc	893.29	K	Joback Method
tf	415.29	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.73	J/mol×K	705.44	Joback Method
cpg	670.30	J/mol×K	736.75	Joback Method
cpg	683.98	J/mol×K	768.06	Joback Method
cpg	696.81	J/mol×K	799.36	Joback Method
cpg	708.85	J/mol×K	830.67	Joback Method
cpg	720.12	J/mol×K	861.98	Joback Method
cpg	730.66	J/mol×K	893.29	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=U355144&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