3-Trifluoromethylbenzoic acid, phenyl ester

Inchi: InChI=1S/C14H9F3O2/c15-14(16,17)11-6-4-5-10(9-11)13(18)19-12-7-2-1-3-8-12/h1-9H
InchiKey: YRDKCSDCXWEWKM-UHFFFAOYSA-N
Formula: C14H9F3O2
SMILES: O=C(Oc1ccccc1)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 266.22

Physical Properties

Property code	Value	Unit	Source
gf	-533.32	kJ/mol	Joback Method
hf	-712.58	kJ/mol	Joback Method
hfus	24.32	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.925		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	648.93	K	Joback Method
tc	872.96	K	Joback Method
tf	389.25	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.47	J/mol×K	648.93	Joback Method
cpg	455.97	J/mol×K	686.27	Joback Method
cpg	468.36	J/mol×K	723.61	Joback Method
cpg	479.70	J/mol×K	760.95	Joback Method
cpg	490.06	J/mol×K	798.29	Joback Method
cpg	499.49	J/mol×K	835.62	Joback Method
cpg	508.07	J/mol×K	872.96	Joback Method

Sources

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=U299038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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