Acetic acid, (4-(trifluoromethoxy)phenyl)methyl ester

Inchi: InChI=1S/C10H9F3O3/c1-7(14)15-6-8-2-4-9(5-3-8)16-10(11,12)13/h2-5H,6H2,1H3
InchiKey: LEOJDDUQYRSCSH-UHFFFAOYSA-N
Formula: C10H9F3O3
SMILES: CC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 234.17
CAS: 102606-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-784.41	kJ/mol	Joback Method
hf	-998.77	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.648		Crippen Method
mcvol	146.620	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1202.00		NIST Webbook
rinpol	1202.00		NIST Webbook
tb	553.15	K	Joback Method
tc	747.14	K	Joback Method
tf	339.98	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.27	J/mol×K	553.15	Joback Method
cpg	364.21	J/mol×K	585.48	Joback Method
cpg	375.47	J/mol×K	617.81	Joback Method
cpg	386.07	J/mol×K	650.15	Joback Method
cpg	396.01	J/mol×K	682.48	Joback Method
cpg	405.32	J/mol×K	714.81	Joback Method
cpg	414.01	J/mol×K	747.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102606995&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