(«alpha»,«alpha»,«alpha»-Trifluoro-p-tolyl)-acetic acid

Other names: 4-Trifluoromethylphenylacetic acid
p-Trifluoromethylphenylacetic acid
Benzeneacetic acid, 4-(trifluoromethyl)-
(«alpha»,«alpha»,«alpha»-trifluoro-4-tolyl)acetic acid

Inchi: InChI=1S/C9H7F3O2/c10-9(11,12)7-3-1-6(2-4-7)5-8(13)14/h1-4H,5H2,(H,13,14)

InchiKey: HNORVZDAANCHAY-UHFFFAOYSA-N

Formula: C9H7F3O2

SMILES: O=C(O)Cc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 204.15

CAS: 32857-62-8

Physical Properties

Property code	Value	Unit	Source
gf	-719.65	kJ/mol	Joback Method
hf	-865.92	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	58.24	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.333		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	577.61	K	Joback Method
tc	765.80	K	Joback Method
tf	345.07	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.99	J/mol×K	577.61	Joback Method
cpg	318.33	J/mol×K	608.98	Joback Method
cpg	327.03	J/mol×K	640.34	Joback Method
cpg	335.13	J/mol×K	671.71	Joback Method
cpg	342.67	J/mol×K	703.07	Joback Method

cpg	349.67	J/mol×K	734.44	Joback Method
cpg	356.17	J/mol×K	765.80	Joback Method

Sources

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=C32857628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume