2,2,2-Trifluoroethylbutyrate

Other names: Butanoic acid, 2,2,2-trifluoroethyl ester
Butyric acid, TFE
Inchi: InChI=1S/C6H9F3O2/c1-2-3-5(10)11-4-6(7,8)9/h2-4H2,1H3
InchiKey: DEXWRCYOMLUJRF-UHFFFAOYSA-N
Formula: C6H9F3O2
SMILES: CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 170.13
CAS: 371-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-815.87	kJ/mol	Joback Method
hf	-1009.05	kJ/mol	Joback Method
hfus	15.91	kJ/mol	Joback Method
hvap	34.36	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.892		Crippen Method
mcvol	108.150	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	385.15 ± 1.50	K	NIST Webbook
tc	568.90	K	Joback Method
tf	233.73	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.81	J/mol×K	407.55	Joback Method
cpg	236.43	J/mol×K	434.44	Joback Method
cpg	245.63	J/mol×K	461.33	Joback Method
cpg	254.43	J/mol×K	488.23	Joback Method
cpg	262.84	J/mol×K	515.12	Joback Method
cpg	270.88	J/mol×K	542.01	Joback Method
cpg	278.54	J/mol×K	568.90	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=C371277&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume