Propionic acid, 2,2-dichloro-3,3,3-trifluoro-, n-butyl ester

Inchi: InChI=1S/C7H9Cl2F3O2/c1-2-3-4-14-5(13)6(8,9)7(10,11)12/h2-4H2,1H3
InchiKey: UEOPJKJKJBWUIQ-UHFFFAOYSA-N
Formula: C7H9Cl2F3O2
SMILES: CCCCOC(=O)C(Cl)(Cl)C(F)(F)F
Mol. weight [g/mol]: 253.05
CAS: 309-23-9

Physical Properties

Property code	Value	Unit	Source
gf	-828.47	kJ/mol	Joback Method
hf	-1069.92	kJ/mol	Joback Method
hfus	19.48	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.066		Crippen Method
mcvol	146.720	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	502.06	K	Joback Method
tc	684.78	K	Joback Method
tf	307.26	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.47	J/mol×K	502.06	Joback Method
cpg	332.96	J/mol×K	532.51	Joback Method
cpg	342.78	J/mol×K	562.97	Joback Method
cpg	351.96	J/mol×K	593.42	Joback Method
cpg	360.53	J/mol×K	623.87	Joback Method
cpg	368.52	J/mol×K	654.33	Joback Method
cpg	375.97	J/mol×K	684.78	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=C309239&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