3-Buten-2-ol, trifluoroacetate

Inchi: InChI=1S/C6H7F3O2/c1-3-4(2)11-5(10)6(7,8)9/h3-4H,1H2,2H3
InchiKey: RHPTZIKNLZAVDC-UHFFFAOYSA-N
Formula: C6H7F3O2
SMILES: C=CC(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 168.11

Physical Properties

Property code	Value	Unit	Source
gf	-730.47	kJ/mol	Joback Method
hf	-888.90	kJ/mol	Joback Method
hfus	11.11	kJ/mol	Joback Method
hvap	33.30	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.666		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	714.60		NIST Webbook
rinpol	714.60		NIST Webbook
tb	403.79	K	Joback Method
tc	572.01	K	Joback Method
tf	216.97	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.93	J/mol×K	403.79	Joback Method
cpg	221.24	J/mol×K	431.83	Joback Method
cpg	230.10	J/mol×K	459.86	Joback Method
cpg	238.52	J/mol×K	487.90	Joback Method
cpg	246.52	J/mol×K	515.94	Joback Method
cpg	254.10	J/mol×K	543.97	Joback Method
cpg	261.29	J/mol×K	572.01	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=U352689&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