3-Buten-1-ol, trifluoroacetate

Inchi: InChI=1S/C6H7F3O2/c1-2-3-4-11-5(10)6(7,8)9/h2H,1,3-4H2
InchiKey: PCRXDGPJDYVEKT-UHFFFAOYSA-N
Formula: C6H7F3O2
SMILES: C=CCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 168.11

Physical Properties

Property code	Value	Unit	Source
gf	-728.03	kJ/mol	Joback Method
hf	-883.62	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	33.69	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.668		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	729.50		NIST Webbook
rinpol	729.50		NIST Webbook
tb	404.23	K	Joback Method
tc	568.76	K	Joback Method
tf	231.97	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.92	J/mol×K	404.23	Joback Method
cpg	220.95	J/mol×K	431.65	Joback Method
cpg	229.54	J/mol×K	459.07	Joback Method
cpg	237.73	J/mol×K	486.49	Joback Method
cpg	245.51	J/mol×K	513.91	Joback Method
cpg	252.90	J/mol×K	541.34	Joback Method
cpg	259.92	J/mol×K	568.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352273&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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