4-Penten-2-ol, 1,1,1-trifluoro-2-(trifluoromethyl)-

Other names: 1,1,1-Trifluoro-2-(trifluoromethyl)pent-4-en-2-ol
Inchi: InChI=1S/C6H6F6O/c1-2-3-4(13,5(7,8)9)6(10,11)12/h2,13H,1,3H2
InchiKey: VHSCQANAKTXZTG-UHFFFAOYSA-N
Formula: C6H6F6O
SMILES: C=CCC(O)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 208.10
CAS: 646-97-9

Physical Properties

Property code	Value	Unit	Source
gf	-1209.68	kJ/mol	Joback Method
hf	-1396.88	kJ/mol	Joback Method
hfus	10.34	kJ/mol	Joback Method
hvap	36.17	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.418		Crippen Method
mcvol	107.590	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	411.47	K	Joback Method
tc	556.65	K	Joback Method
tf	227.24	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.42	J/mol×K	411.47	Joback Method
cpg	258.00	J/mol×K	435.67	Joback Method
cpg	266.96	J/mol×K	459.86	Joback Method
cpg	275.32	J/mol×K	484.06	Joback Method
cpg	283.12	J/mol×K	508.26	Joback Method
cpg	290.39	J/mol×K	532.45	Joback Method
cpg	297.16	J/mol×K	556.65	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=C646979&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