2,2,3,3-Tetrafluoro-1,4-butanediol

Inchi: InChI=1S/C4H6F4O2/c5-3(6,1-9)4(7,8)2-10/h9-10H,1-2H2
InchiKey: CDZXJJOGDCLNKX-UHFFFAOYSA-N
Formula: C4H6F4O2
SMILES: OCC(F)(F)C(F)(F)CO
Mol. weight [g/mol]: 162.08
CAS: 425-61-6

Physical Properties

Property code	Value	Unit	Source
gf	-1064.40	kJ/mol	Joback Method
hf	-1232.29	kJ/mol	Joback Method
hfus	11.78	kJ/mol	Joback Method
hvap	52.00	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.242		Crippen Method
mcvol	86.040	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	359.00 ± 1.00	K	NIST Webbook
tc	613.16	K	Joback Method
tf	263.68	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.34	J/mol×K	465.90	Joback Method
cpg	219.92	J/mol×K	490.44	Joback Method
cpg	226.10	J/mol×K	514.99	Joback Method
cpg	231.89	J/mol×K	539.53	Joback Method
cpg	237.32	J/mol×K	564.08	Joback Method
cpg	242.40	J/mol×K	588.62	Joback Method
cpg	247.15	J/mol×K	613.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C425616&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume