Promoxolane

Inchi: InChI=1S/C10H20O3/c1-7(2)10(8(3)4)12-6-9(5-11)13-10/h7-9,11H,5-6H2,1-4H3
InchiKey: HHFOOWPWAXNJNY-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CC(C)C1(C(C)C)OCC(CO)O1
Mol. weight [g/mol]: 188.26
CAS: 470-43-9

Physical Properties

Property code	Value	Unit	Source
gf	-257.27	kJ/mol	Joback Method
hf	-621.14	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	61.57	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.402		Crippen Method
mcvol	158.510	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	584.25	K	Joback Method
tc	776.79	K	Joback Method
tf	316.98	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.84	J/mol×K	584.25	Joback Method
cpg	447.96	J/mol×K	616.34	Joback Method
cpg	462.31	J/mol×K	648.43	Joback Method
cpg	475.95	J/mol×K	680.52	Joback Method
cpg	488.98	J/mol×K	712.61	Joback Method
cpg	501.47	J/mol×K	744.70	Joback Method
cpg	513.51	J/mol×K	776.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C470439&Units=SI

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