Isolyratol

Inchi: InChI=1S/C10H16O/c1-6-9(7(2)3)10(11)8(4)5/h6,9-11H,1-2,4H2,3,5H3
InchiKey: YAATZFSMWSSRHJ-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=CC(C(=C)C)C(O)C(=C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	138.04	kJ/mol	Joback Method
hf	-55.81	kJ/mol	Joback Method
hfus	12.24	kJ/mol	Joback Method
hvap	51.91	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.302		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1052.00		NIST Webbook
rinpol	1053.00		NIST Webbook
ripol	1524.00		NIST Webbook
tb	509.30	K	Joback Method
tc	688.27	K	Joback Method
tf	200.08	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.11	J/mol×K	509.30	Joback Method
cpg	337.66	J/mol×K	539.13	Joback Method
cpg	349.59	J/mol×K	568.96	Joback Method
cpg	360.92	J/mol×K	598.79	Joback Method
cpg	371.67	J/mol×K	628.62	Joback Method
cpg	381.89	J/mol×K	658.45	Joback Method
cpg	391.59	J/mol×K	688.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591067&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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