

Costic acid

Inchi:	InChI=1S/C15H22O2/c1-10-5-4-7-15(3)8-6-12(9-13(10)15)11(2)14(16)17/h12-13H,1-2,4-
InchiKey:	UJQGVNDNQDFTTLZ-YOYPFHDYSA-N
Formula:	C15H22O2
SMILES:	<chem>C=C(C(=O)O)C1CCC2(C)CCCC(=C)C2C1</chem>
Mol. weight [g/mol]:	234.33
CAS:	3650-43-9

Physical Properties

Property code	Value	Unit	Source
gf	1.95	kJ/mol	Joback Method
hf	-302.00	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	71.03	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.790		Crippen Method
mvol	199.330	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1862.00		NIST Webbook
tb	710.50	K	Joback Method
tc	924.17	K	Joback Method
tf	408.98	K	Joback Method
vc	0.746	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.29	J/molxK	710.50	Joback Method
cpg	611.87	J/molxK	746.11	Joback Method
cpg	628.60	J/molxK	781.72	Joback Method
cpg	644.62	J/molxK	817.33	Joback Method
cpg	660.07	J/molxK	852.94	Joback Method
cpg	675.08	J/molxK	888.55	Joback Method
cpg	689.79	J/molxK	924.17	Joback Method

Sources

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=C3650439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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