Oxepine, 2,7-dimethyl-

Inchi: InChI=1S/C8H10O/c1-7-5-3-4-6-8(2)9-7/h3-6H,1-2H3
InchiKey: SFVUIUUSVAMYPP-UHFFFAOYSA-N
Formula: C8H10O
SMILES: CC1=CC=CC=C(C)O1
Mol. weight [g/mol]: 122.16
CAS: 1487-99-6

Physical Properties

Property code	Value	Unit	Source
gf	21.04	kJ/mol	Joback Method
hf	-121.55	kJ/mol	Joback Method
hfus	16.01	kJ/mol	Joback Method
hvap	41.02	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.380		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	916.70		NIST Webbook
rinpol	916.70		NIST Webbook
rinpol	916.70		NIST Webbook
rinpol	934.00		NIST Webbook
tb	445.32	K	Joback Method
tc	664.62	K	Joback Method
tf	241.91	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.66	J/mol×K	445.32	Joback Method
cpg	260.15	J/mol×K	628.07	Joback Method
cpg	249.93	J/mol×K	591.52	Joback Method

cpg	239.08	J/mol×K	554.97	Joback Method
cpg	227.60	J/mol×K	518.42	Joback Method
cpg	215.46	J/mol×K	481.87	Joback Method
cpg	269.76	J/mol×K	664.62	Joback Method
dvisc	0.0002173	Pa×s	445.32	Joback Method
dvisc	0.0002860	Pa×s	411.42	Joback Method
dvisc	0.0003956	Pa×s	377.52	Joback Method
dvisc	0.0005834	Pa×s	343.62	Joback Method
dvisc	0.0009366	Pa×s	309.71	Joback Method
dvisc	0.0016893	Pa×s	275.81	Joback Method
dvisc	0.0035946	Pa×s	241.91	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1487996&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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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