

Oxirane, hexyl-

Other names:	Octane, 1,2-epoxy- «alpha»-Epoxyoctane n-Octene-1,2-oxide Hexyloxirane Octane 1,2-oxide Octene-1,2-oxide 1-Octene epoxide 1-Octene oxide 1,2-Epoxy-n-octane 1,2-Epoxyoctane Octylene epoxide 1,2-Epoxyoktan Oktylenoxid n-Hexyloxirane 2-Hexyloxirane 1,2-Octylene oxide NSC 24246
Inchi:	InChI=1S/C8H16O/c1-2-3-4-5-6-8-7-9-8/h8H,2-7H2,1H3
InchiKey:	NJWSNNWLBMXQR-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CCCCCCC1CO1
Mol. weight [g/mol]:	128.21
CAS:	2984-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-8.89	kJ/mol	Joback Method
hf	-267.65	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	37.83	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.356		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	416.13	K	Joback Method
tc	594.55	K	Joback Method
tf	224.43	K	Joback Method

vc

0.462

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.71	J/mol×K	416.13	Joback Method
cpg	261.88	J/mol×K	445.87	Joback Method
cpg	275.37	J/mol×K	475.60	Joback Method
cpg	288.21	J/mol×K	505.34	Joback Method
cpg	300.43	J/mol×K	535.07	Joback Method
cpg	312.05	J/mol×K	564.81	Joback Method
cpg	323.10	J/mol×K	594.55	Joback Method
dvisc	0.0022201	Paxs	224.43	Joback Method
dvisc	0.0014439	Paxs	256.38	Joback Method
dvisc	0.0010330	Paxs	288.33	Joback Method
dvisc	0.0007901	Paxs	320.28	Joback Method
dvisc	0.0006345	Paxs	352.23	Joback Method
dvisc	0.0005284	Paxs	384.18	Joback Method
dvisc	0.0004526	Paxs	416.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.00	K	2.30	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2984501&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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