

2,3-Epoxy-2,4,4-trimethyl pentane

Inchi:	InChI=1S/C8H16O/c1-7(2,3)6-8(4,5)9-6/h6H,1-5H3
InchiKey:	OUYYZNFRPHQCIM-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CC(C)(C)C1OC1(C)C
Mol. weight [g/mol]:	128.21
CAS:	96-06-0

Physical Properties

Property code	Value	Unit	Source
gf	-19.25	kJ/mol	Joback Method
hf	-281.50	kJ/mol	Joback Method
hfus	9.95	kJ/mol	Joback Method
hvap	35.07	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.210		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	408.47	K	Joback Method
tc	606.86	K	Joback Method
tf	246.51	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.25	J/molxK	408.47	Joback Method
cpg	266.99	J/molxK	441.53	Joback Method
cpg	282.45	J/molxK	474.60	Joback Method
cpg	296.75	J/molxK	507.66	Joback Method
cpg	310.00	J/molxK	540.73	Joback Method
cpg	322.31	J/molxK	573.79	Joback Method
cpg	333.80	J/molxK	606.86	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=C96060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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