

Exo-2-isobutylidenetetrahydrofuran

Inchi:	InChI=1S/C8H14O/c1-7(2)6-8-4-3-5-9-8/h6-7H,3-5H2,1-2H3/b8-6+
InchiKey:	JACGTRYVOSXWIR-SOFGYWHQSA-N
Formula:	C8H14O
SMILES:	CC(C)C=C1CCCO1
Mol. weight [g/mol]:	126.20
CAS:	56755-30-7

Physical Properties

Property code	Value	Unit	Source
gf	17.64	kJ/mol	Joback Method
hf	-188.88	kJ/mol	Joback Method
hfus	14.12	kJ/mol	Joback Method
hvap	38.88	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.337		Crippen Method
mvol	114.290	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	435.54	K	Joback Method
tc	641.22	K	Joback Method
tf	216.99	K	Joback Method
vc	0.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.16	J/molxK	435.54	Joback Method
cpg	247.10	J/molxK	469.82	Joback Method
cpg	261.22	J/molxK	504.10	Joback Method
cpg	274.55	J/molxK	538.38	Joback Method
cpg	287.13	J/molxK	572.66	Joback Method
cpg	298.99	J/molxK	606.94	Joback Method
cpg	310.17	J/molxK	641.22	Joback Method
dvisc	0.0070769	Paxs	216.99	Joback Method
dvisc	0.0028444	Paxs	253.41	Joback Method

dvisc	0.0014376	Paxs	289.84	Joback Method
dvisc	0.0008462	Paxs	326.26	Joback Method
dvisc	0.0005540	Paxs	362.69	Joback Method
dvisc	0.0003919	Paxs	399.11	Joback Method
dvisc	0.0002937	Paxs	435.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56755307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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