Oxetane, 3,3-dibutyl

Inchi: InChI=1S/C11H22O/c1-3-5-7-11(8-6-4-2)9-12-10-11/h3-10H2,1-2H3
InchiKey: ISNIPFKDIOZFHP-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCCCC1(CCCC)COC1
Mol. weight [g/mol]: 170.29

Physical Properties

Property code	Value	Unit	Source
gf	-1.22	kJ/mol	Joback Method
hf	-320.49	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hvap	43.52	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.383		Crippen Method
mcvol	160.860	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
tb	489.28	K	Joback Method
tc	677.09	K	Joback Method
tf	278.62	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.22	J/mol×K	489.28	Joback Method
cpg	398.92	J/mol×K	520.58	Joback Method
cpg	415.60	J/mol×K	551.88	Joback Method
cpg	431.35	J/mol×K	583.19	Joback Method
cpg	446.26	J/mol×K	614.49	Joback Method
cpg	460.41	J/mol×K	645.79	Joback Method
cpg	473.90	J/mol×K	677.09	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=R6581&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume