2-Butyl-1,3-oxothiolane

Inchi: InChI=1S/C7H14OS/c1-2-3-4-7-8-5-6-9-7/h7H,2-6H2,1H3
InchiKey: GLHSHWIEAQNAAO-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCCCC1OCCS1
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	-1.65	kJ/mol	Joback Method
hf	-214.07	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	41.75	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.266		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1109.00		NIST Webbook
tb	449.62	K	Joback Method
tc	659.72	K	Joback Method
tf	289.57	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.50	J/mol×K	449.62	Joback Method
cpg	266.49	J/mol×K	484.64	Joback Method

cpg	280.68	J/mol×K	519.65	Joback Method
cpg	294.09	J/mol×K	554.67	Joback Method
cpg	306.76	J/mol×K	589.69	Joback Method
cpg	318.72	J/mol×K	624.71	Joback Method
cpg	329.99	J/mol×K	659.72	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R78791&Units=SI

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