2-Butylidene-1,3-dithiolane

Inchi: InChI=1S/C7H12S2/c1-2-3-4-7-8-5-6-9-7/h4H,2-3,5-6H2,1H3
InchiKey: VLAHDRRAZZBLEP-UHFFFAOYSA-N
Formula: C7H12S2
SMILES: CCCC=C1SCCS1
Mol. weight [g/mol]: 160.30

Physical Properties

Property code	Value	Unit	Source
gf	177.50	kJ/mol	Joback Method
hf	59.56	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.108		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
tb	481.81	K	Joback Method
tc	716.22	K	Joback Method
tf	361.05	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.88	J/mol×K	481.81	Joback Method
cpg	264.58	J/mol×K	520.88	Joback Method
cpg	277.36	J/mol×K	559.95	Joback Method
cpg	289.30	J/mol×K	599.02	Joback Method
cpg	300.43	J/mol×K	638.08	Joback Method
cpg	310.83	J/mol×K	677.15	Joback Method
cpg	320.54	J/mol×K	716.22	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=R391090&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