4-Methyl-2-propyl-1,3-dithiolane

Other names: 2-propyl-4-methyl-1,3-dithiolane
Inchi: InChI=1S/C7H14S2/c1-3-4-7-8-5-6(2)9-7/h6-7H,3-5H2,1-2H3
InchiKey: QTQGHUYMHBCNSH-UHFFFAOYSA-N
Formula: C7H14S2
SMILES: CCCC1SCC(C)S1
Mol. weight [g/mol]: 162.32

Physical Properties

Property code	Value	Unit	Source
gf	116.62	kJ/mol	Joback Method
hf	-57.15	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	42.75	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.981		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1270.00		NIST Webbook
tb	465.83	K	Joback Method
tc	691.45	K	Joback Method
tf	342.21	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.62	J/mol×K	465.83	Joback Method
cpg	284.49	J/mol×K	503.43	Joback Method

cpg	299.47	J/mol×K	541.04	Joback Method
cpg	313.60	J/mol×K	578.64	Joback Method
cpg	326.90	J/mol×K	616.25	Joback Method
cpg	339.41	J/mol×K	653.85	Joback Method
cpg	351.16	J/mol×K	691.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78915&Units=SI
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

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