7-butyloxepane-2-thione

Inchi: InChI=1S/C10H18OS/c1-2-3-6-9-7-4-5-8-10(12)11-9/h9H,2-8H2,1H3
InchiKey: MCAXROCTXJWOCL-UHFFFAOYSA-N
Formula: C10H18OS
SMILES: CCCCC1CCCCC(=S)O1
Mol. weight [g/mol]: 186.31

Physical Properties

Property code	Value	Unit	Source
gf	50.40	kJ/mol	Joback Method
hf	-218.47	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.463		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
ripol	2288.00		NIST Webbook
ripol	2288.00		NIST Webbook
tb	551.61	K	Joback Method
tc	774.57	K	Joback Method
tf	296.56	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.69	J/mol×K	551.61	Joback Method
cpg	397.65	J/mol×K	588.77	Joback Method
cpg	414.52	J/mol×K	625.93	Joback Method
cpg	430.35	J/mol×K	663.09	Joback Method
cpg	445.17	J/mol×K	700.25	Joback Method
cpg	459.04	J/mol×K	737.41	Joback Method

cpg	472.00	J/mol×K	774.57	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=R422570&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume