n-Butyl n-hexyl disulfide

Other names: Butyl hexyl disulfide
Inchi: InChI=1S/C10H22S2/c1-3-5-7-8-10-12-11-9-6-4-2/h3-10H2,1-2H3
InchiKey: AQCMTUGVHLFFKR-UHFFFAOYSA-N
Formula: C10H22S2
SMILES: CCCCCCSSCCCC
Mol. weight [g/mol]: 206.41
CAS: 64580-57-0

Physical Properties

Property code	Value	Unit	Source
gf	99.56	kJ/mol	Joback Method
hf	-165.99	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	51.49	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.748		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
ripol	1746.00		NIST Webbook
tb	565.76	K	Joback Method
tc	765.78	K	Joback Method
tf	271.26	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.05	J/mol×K	565.76	Joback Method
cpg	451.18	J/mol×K	599.10	Joback Method
cpg	466.54	J/mol×K	632.43	Joback Method
cpg	481.15	J/mol×K	665.77	Joback Method
cpg	495.01	J/mol×K	699.11	Joback Method
cpg	508.14	J/mol×K	732.45	Joback Method
cpg	520.55	J/mol×K	765.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64580570&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume