Benzene, (2-butenylthio)-, (Z)-

Inchi: InChI=1S/C10H12S/c1-2-3-9-11-10-7-5-4-6-8-10/h2-8H,9H2,1H3/b3-2-
InchiKey: BNNLEMHAUPCSCL-IHWYPQMZSA-N
Formula: C10H12S
SMILES: CC=CCSc1ccccc1
Mol. weight [g/mol]: 164.27
CAS: 36195-55-8

Physical Properties

Property code	Value	Unit	Source
gf	259.07	kJ/mol	Joback Method
hf	145.89	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.355		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	527.82	K	Joback Method
tc	765.27	K	Joback Method
tf	258.20	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.46	J/mol×K	527.82	Joback Method
cpg	306.31	J/mol×K	567.40	Joback Method
cpg	320.13	J/mol×K	606.97	Joback Method
cpg	332.95	J/mol×K	646.55	Joback Method
cpg	344.83	J/mol×K	686.12	Joback Method
cpg	355.84	J/mol×K	725.70	Joback Method
cpg	366.03	J/mol×K	765.27	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=C36195558&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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