

Sulfone, p-nonylphenyl-2,3,3-tribromoallyl-

Inchi:	InChI=1S/C18H25Br3O2S/c1-2-3-4-5-6-7-8-9-15-10-12-16(13-11-15)24(22,23)14-17(19)
InchiKey:	RTZOATNWOWLQMY-UHFFFAOYSA-N
Formula:	C18H25Br3O2S
SMILES:	CCCCCCCCCc1ccc(S(=O)(=O)CC(Br)=C(Br)Br)cc1
Mol. weight [g/mol]:	545.17
CAS:	116295-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-159.00	kJ/mol	Joback Method
hf	-466.51	kJ/mol	Joback Method
hfus	60.84	kJ/mol	Joback Method
hvap	96.66	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.107		Crippen Method
mcvol	317.010	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
tb	893.08	K	Joback Method
tc	1117.62	K	Joback Method
tf	516.52	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.92	J/molxK	893.08	Joback Method
cpg	868.65	J/molxK	930.50	Joback Method
cpg	881.44	J/molxK	967.93	Joback Method
cpg	893.38	J/molxK	1005.35	Joback Method
cpg	904.56	J/molxK	1042.77	Joback Method
cpg	915.07	J/molxK	1080.20	Joback Method
cpg	925.01	J/molxK	1117.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116295717&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
mccvol:	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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