2,4,6-Tri-isopropyl-[1,3,5]trithiane

Inchi: InChI=1S/C12H24S3/c1-7(2)10-13-11(8(3)4)15-12(14-10)9(5)6/h7-12H,1-6H3
InchiKey: GZIFOGZGZSUARX-UHFFFAOYSA-N
Formula: C12H24S3
SMILES: CC(C)C1SC(C(C)C)SC(C(C)C)S1
Mol. weight [g/mol]: 264.51

Physical Properties

Property code	Value	Unit	Source
gf	171.45	kJ/mol	Joback Method
hf	-157.43	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	58.39	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.146		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
ripol	2070.00		NIST Webbook
tb	626.34	K	Joback Method
tc	866.40	K	Joback Method
tf	429.25	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.71	J/mol×K	626.34	Joback Method
cpg	584.79	J/mol×K	666.35	Joback Method
cpg	605.45	J/mol×K	706.36	Joback Method
cpg	624.72	J/mol×K	746.37	Joback Method
cpg	642.65	J/mol×K	786.38	Joback Method
cpg	659.28	J/mol×K	826.39	Joback Method
cpg	674.66	J/mol×K	866.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495088&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

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