probucol

Other names: 4,4'-(propane-2,2-diylbis(sulfanediyl))bis(2,6-di-tert-butylphenol)
Inchi: InChI=1S/C31H48O2S2/c1-27(2,3)21-15-19(16-22(25(21)32)28(4,5)6)34-31(13,14)35-20
InchiKey: FYPMFJGVHOHGLL-UHFFFAOYSA-N
Formula: C31H48O2S2
SMILES: CC(C)(Sc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1)Sc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 516.86

Physical Properties

Property code	Value	Unit	Source
gf	167.64	kJ/mol	Joback Method
hf	-570.62	kJ/mol	Joback Method
hfus	31.99	kJ/mol	The slow molecular dynamics in amorphous probucol
hvap	124.98	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	9.908		Crippen Method
mcvol	444.570	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
tb	1264.61	K	Joback Method
tc	1550.25	K	Joback Method
tf	399.05	K	The slow molecular dynamics in amorphous probucol
tt	298.15	K	The slow molecular dynamics in amorphous probucol
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1648.21	J/mol×K	1264.61	Joback Method
cpg	1685.33	J/mol×K	1312.22	Joback Method
cpg	1725.69	J/mol×K	1359.82	Joback Method
cpg	1769.85	J/mol×K	1407.43	Joback Method

cpg	1818.39	J/mol×K	1455.04	Joback Method
cpg	1871.88	J/mol×K	1502.65	Joback Method
cpg	1930.89	J/mol×K	1550.25	Joback Method

Sources

The slow molecular dynamics in amorphous probucol:	https://www.doi.org/10.1016/j.tca.2014.09.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
tt:	Triple Point Temperature
vc:	Critical Volume