Febutol

Inchi: InChI=1S/C32H48O2S2/c1-19(2)28(35-20-15-22(29(3,4)5)26(33)23(16-20)30(6,7)8)36-2
InchiKey: IMLBXHMGSBYKDH-UHFFFAOYSA-N
Formula: C32H48O2S2
SMILES: CC(C)=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]: 528.85

Physical Properties

Property code	Value	Unit	Source
gf	236.34	kJ/mol	Joback Method
hf	-484.87	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	128.62	kJ/mol	Joback Method
log10ws	-10.64		Crippen Method
logp	10.424		Crippen Method
mcvol	454.360	ml/mol	McGowan Method
pc	965.67	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	1294.64	K	Joback Method
tc	1585.49	K	Joback Method
tf	822.24	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1696.12	J/mol×K	1294.64	Joback Method
cpg	1736.85	J/mol×K	1343.12	Joback Method
cpg	1781.30	J/mol×K	1391.59	Joback Method
cpg	1830.04	J/mol×K	1440.07	Joback Method
cpg	1883.69	J/mol×K	1488.54	Joback Method
cpg	1942.82	J/mol×K	1537.02	Joback Method
cpg	2008.04	J/mol×K	1585.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R38939&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume