Benzenesulfonic acid, 4-methyl-, 2-methylpropyl ester

Other names: Isobutyl 4-methylbenzenesulfonate
Inchi: InChI=1S/C11H16O3S/c1-9(2)8-14-15(12,13)11-6-4-10(3)5-7-11/h4-7,9H,8H2,1-3H3
InchiKey: QIMRPGAQCKHRKB-UHFFFAOYSA-N
Formula: C11H16O3S
SMILES: Cc1ccc(S(=O)(=O)OCC(C)C)cc1
Mol. weight [g/mol]: 228.31
CAS: 4873-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-431.46	kJ/mol	Joback Method
hf	-636.16	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.356		Crippen Method
mcvol	176.050	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
tb	552.50	K	Joback Method
tc	751.81	K	Joback Method
tf	298.46	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.05	J/mol×K	552.50	Joback Method
cpg	424.75	J/mol×K	585.72	Joback Method
cpg	439.65	J/mol×K	618.94	Joback Method
cpg	453.75	J/mol×K	652.15	Joback Method
cpg	467.05	J/mol×K	685.37	Joback Method
cpg	479.56	J/mol×K	718.59	Joback Method

cpg	491.26	J/mol×K	751.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4873567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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