isopropyl benzyl sulfide

Inchi: InChI=1S/C10H14S/c1-9(2)11-8-10-6-4-3-5-7-10/h3-7,9H,8H2,1-2H3
InchiKey: GGIZKZIRURGXOI-UHFFFAOYSA-N
Formula: C10H14S
SMILES: CC(C)SCc1ccccc1
Mol. weight [g/mol]: 166.28

Physical Properties

Property code	Value	Unit	Source
gf	176.41	kJ/mol	Joback Method
hf	23.39	kJ/mol	Joback Method
hfus	16.30	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.328		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	523.22	K	Joback Method
tc	754.96	K	Joback Method
tf	248.28	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.00	J/mol×K	523.22	Joback Method
cpg	325.83	J/mol×K	561.84	Joback Method
cpg	340.66	J/mol×K	600.47	Joback Method
cpg	354.52	J/mol×K	639.09	Joback Method
cpg	367.45	J/mol×K	677.71	Joback Method
cpg	379.48	J/mol×K	716.34	Joback Method
cpg	390.65	J/mol×K	754.96	Joback Method

Sources

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=R157716&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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