Benzoic acid, 2-(methylthio)-, neopentyl ester

Inchi: InChI=1S/C13H18O2S/c1-13(2,3)9-15-12(14)10-7-5-6-8-11(10)16-4/h5-8H,9H2,1-4H3
InchiKey: LSOOISSPNCXVFI-UHFFFAOYSA-N
Formula: C13H18O2S
SMILES: CSc1ccccc1C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 238.35

Physical Properties

Property code	Value	Unit	Source
gf	-36.60	kJ/mol	Joback Method
hf	-298.27	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	62.15	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.611		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1802.00		NIST Webbook
tb	670.34	K	Joback Method
tc	902.69	K	Joback Method
tf	384.19	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.26	J/mol×K	670.34	Joback Method
cpg	518.19	J/mol×K	709.06	Joback Method
cpg	532.97	J/mol×K	747.79	Joback Method
cpg	546.64	J/mol×K	786.51	Joback Method
cpg	559.24	J/mol×K	825.24	Joback Method
cpg	570.82	J/mol×K	863.96	Joback Method
cpg	581.42	J/mol×K	902.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375370&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume