2-(Methylthio)benzoic acid, 2-propylpentyl ester

Inchi: InChI=1S/C16H24O2S/c1-4-8-13(9-5-2)12-18-16(17)14-10-6-7-11-15(14)19-3/h6-7,10-11

InchiKey: DXBSTOAFUPWBMU-UHFFFAOYSA-N

Formula: C16H24O2S

SMILES: CCCC(CCC)COC(=O)c1ccccc1SC

Mol. weight [g/mol]: 280.43

Physical Properties

Property code	Value	Unit	Source
gf	-16.62	kJ/mol	Joback Method
hf	-356.72	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.782		Crippen Method
mcvol	236.330	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2109.00		NIST Webbook
tb	741.77	K	Joback Method
tc	955.49	K	Joback Method
tf	400.58	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.26	J/mol×K	741.77	Joback Method
cpg	677.93	J/mol×K	777.39	Joback Method
cpg	693.50	J/mol×K	813.01	Joback Method
cpg	707.97	J/mol×K	848.63	Joback Method
cpg	721.38	J/mol×K	884.25	Joback Method
cpg	733.74	J/mol×K	919.87	Joback Method
cpg	745.09	J/mol×K	955.49	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=U374940&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