Sebacic acid, 4-methylthiobenzyl propyl ester

Inchi: InChI=1S/C20H30O4S/c1-3-16-23-19(21)10-8-6-4-5-7-9-11-20(22)24-17-12-14-18(25-2)1
InchiKey: FFCTXSVWPXVVEA-UHFFFAOYSA-N
Formula: C20H30O4S
SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 366.51

Physical Properties

Property code	Value	Unit	Source
gf	-214.42	kJ/mol	Joback Method
hf	-678.80	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.388		Crippen Method
mcvol	300.130	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tb	910.02	K	Joback Method
tc	1123.46	K	Joback Method
tf	532.82	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.75	J/mol×K	910.02	Joback Method
cpg	951.39	J/mol×K	945.59	Joback Method
cpg	964.69	J/mol×K	981.17	Joback Method
cpg	976.70	J/mol×K	1016.74	Joback Method
cpg	987.41	J/mol×K	1052.31	Joback Method
cpg	996.85	J/mol×K	1087.89	Joback Method
cpg	1005.05	J/mol×K	1123.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380642&Units=SI

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