Sebacic acid, hexyl 4-methylthiobenzyl ester

Inchi: InChI=1S/C23H36O4S/c1-3-4-5-12-19-26-22(24)13-10-8-6-7-9-11-14-23(25)27-20-15-17
InchiKey: KUHBLHXDDPMPEF-UHFFFAOYSA-N
Formula: C23H36O4S
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 408.60

Physical Properties

Property code	Value	Unit	Source
gf	-189.16	kJ/mol	Joback Method
hf	-740.72	kJ/mol	Joback Method
hfus	58.68	kJ/mol	Joback Method
hvap	94.86	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.558		Crippen Method
mcvol	342.400	ml/mol	McGowan Method
pc	1110.37	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	978.66	K	Joback Method
tc	1199.12	K	Joback Method
tf	566.63	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.15	J/mol×K	978.66	Joback Method
cpg	1132.04	J/mol×K	1015.40	Joback Method
cpg	1145.41	J/mol×K	1052.15	Joback Method
cpg	1157.30	J/mol×K	1088.89	Joback Method
cpg	1167.73	J/mol×K	1125.64	Joback Method
cpg	1176.73	J/mol×K	1162.38	Joback Method
cpg	1184.33	J/mol×K	1199.12	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=U380646&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