Sebacic acid, 4-methylthiobenzyl pentyl ester

Inchi: InChI=1S/C22H34O4S/c1-3-4-11-18-25-21(23)12-9-7-5-6-8-10-13-22(24)26-19-14-16-20
InchiKey: CVGOLIAQXQNMCC-UHFFFAOYSA-N
Formula: C22H34O4S
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(SC)cc1
Mol. weight [g/mol]: 394.57

Physical Properties

Property code	Value	Unit	Source
gf	-197.58	kJ/mol	Joback Method
hf	-720.08	kJ/mol	Joback Method
hfus	56.09	kJ/mol	Joback Method
hvap	92.63	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.168		Crippen Method
mcvol	328.310	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	955.78	K	Joback Method
tc	1173.00	K	Joback Method
tf	555.36	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1056.50	J/mol×K	955.78	Joback Method
cpg	1071.31	J/mol×K	991.98	Joback Method
cpg	1084.67	J/mol×K	1028.19	Joback Method
cpg	1096.61	J/mol×K	1064.39	Joback Method
cpg	1107.16	J/mol×K	1100.59	Joback Method
cpg	1116.34	J/mol×K	1136.80	Joback Method
cpg	1124.19	J/mol×K	1173.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380645&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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