Sebacic acid, isobutyl 4-methylthiobenzyl ester

Inchi: InChI=1S/C21H32O4S/c1-17(2)16-24-20(22)10-8-6-4-5-7-9-11-21(23)25-18-12-14-19(26

InchiKey: VKBHWUVEXHEELX-UHFFFAOYSA-N

Formula: C21H32O4S

SMILES: CSc1ccc(OC(=O)CCCCCCCCCC(=O)OCC(C)C)cc1

Mol. weight [g/mol]: 380.54

Physical Properties

Property code	Value	Unit	Source
gf	-208.44	kJ/mol	Joback Method
hf	-704.72	kJ/mol	Joback Method
hfus	49.98	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.634		Crippen Method
mcvol	314.220	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	2913.00		NIST Webbook
rinpol	2913.00		NIST Webbook
tb	932.46	K	Joback Method
tc	1148.64	K	Joback Method
tf	529.09	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.81	J/mol×K	932.46	Joback Method
cpg	1011.58	J/mol×K	968.49	Joback Method
cpg	1024.94	J/mol×K	1004.52	Joback Method
cpg	1036.91	J/mol×K	1040.55	Joback Method
cpg	1047.51	J/mol×K	1076.58	Joback Method
cpg	1056.77	J/mol×K	1112.61	Joback Method
cpg	1064.72	J/mol×K	1148.64	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=U380643&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