Sebacic acid, isobutyl 2-methoxybenzyl ester

Inchi: InChI=1S/C22H34O5/c1-18(2)16-26-21(23)14-8-6-4-5-7-9-15-22(24)27-17-19-12-10-11-1
InchiKey: VQPPLCUWSPBVPD-UHFFFAOYSA-N
Formula: C22H34O5
SMILES: COc1ccccc1COC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-338.14	kJ/mol	Joback Method
hf	-899.45	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	87.84	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.058		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2748.00		NIST Webbook
tb	908.98	K	Joback Method
tc	1115.86	K	Joback Method
tf	528.19	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.47	J/mol×K	908.98	Joback Method
cpg	1043.51	J/mol×K	943.46	Joback Method
cpg	1058.17	J/mol×K	977.94	Joback Method
cpg	1071.48	J/mol×K	1012.42	Joback Method
cpg	1083.45	J/mol×K	1046.90	Joback Method
cpg	1094.10	J/mol×K	1081.38	Joback Method
cpg	1103.44	J/mol×K	1115.86	Joback Method
dvisc	0.0003727	Pa×s	528.19	Joback Method
dvisc	0.0001922	Pa×s	591.65	Joback Method

dvisc	0.0001127	Pa×s	655.12	Joback Method
dvisc	0.0000726	Pa×s	718.59	Joback Method
dvisc	0.0000503	Pa×s	782.05	Joback Method
dvisc	0.0000367	Pa×s	845.51	Joback Method
dvisc	0.0000281	Pa×s	908.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380772&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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