Sebacic acid, 2-methoxybenzyl propyl ester

Inchi: InChI=1S/C21H32O5/c1-3-16-25-20(22)14-8-6-4-5-7-9-15-21(23)26-17-18-12-10-11-13-1
InchiKey: ICERVUMVKHMWHN-UHFFFAOYSA-N
Formula: C21H32O5
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1OC
Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-344.12	kJ/mol	Joback Method
hf	-873.53	kJ/mol	Joback Method
hfus	50.56	kJ/mol	Joback Method
hvap	86.00	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.812		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2693.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1089.96	K	Joback Method
tf	531.92	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.74	J/mol×K	886.54	Joback Method
cpg	1033.23	J/mol×K	1056.05	Joback Method
cpg	1022.43	J/mol×K	1022.15	Joback Method
cpg	1010.40	J/mol×K	988.25	Joback Method
cpg	997.11	J/mol×K	954.35	Joback Method
cpg	982.57	J/mol×K	920.44	Joback Method
cpg	1042.80	J/mol×K	1089.96	Joback Method
dvisc	0.0000356	Pa×s	886.54	Joback Method
dvisc	0.0000458	Pa×s	827.44	Joback Method

dvisc	0.0000612	Pa×s	768.33	Joback Method
dvisc	0.0000860	Pa×s	709.23	Joback Method
dvisc	0.0001284	Pa×s	650.13	Joback Method
dvisc	0.0002078	Pa×s	591.02	Joback Method
dvisc	0.0003742	Pa×s	531.92	Joback Method

Sources

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=U380771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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