Sebacic acid, di(2-(2-methoxyethyl)heptyl) ester

Inchi: InChI=1S/C30H58O6/c1-5-7-13-17-27(21-23-33-3)25-35-29(31)19-15-11-9-10-12-16-20-

InchiKey: LCVJSTOXOYCXBW-UHFFFAOYSA-N

Formula: C30H58O6

SMILES: CCCCCC(CCOC)COC(=O)CCCCCCCCC(=O)OCC(CCCCC)CCOC

Mol. weight [g/mol]: 514.78

Physical Properties

Property code	Value	Unit	Source
gf	-481.00	kJ/mol	Joback Method
hf	-1427.13	kJ/mol	Joback Method
hfus	74.36	kJ/mol	Joback Method
hvap	104.73	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	7.660		Crippen Method
mcvol	460.180	ml/mol	McGowan Method
pc	617.57	kPa	Joback Method
rinpol	3422.00		NIST Webbook
rinpol	3422.00		NIST Webbook
tb	1082.34	K	Joback Method
tc	1371.18	K	Joback Method
tf	586.64	K	Joback Method
vc	1.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1665.21	J/mol×K	1082.34	Joback Method
cpg	1686.60	J/mol×K	1130.48	Joback Method
cpg	1704.42	J/mol×K	1178.62	Joback Method
cpg	1718.76	J/mol×K	1226.76	Joback Method
cpg	1729.67	J/mol×K	1274.90	Joback Method
cpg	1737.24	J/mol×K	1323.04	Joback Method
cpg	1741.53	J/mol×K	1371.18	Joback Method
dvisc	0.0001314	Pa×s	586.64	Joback Method

dvisc	0.0000544	Pa×s	669.26	Joback Method
dvisc	0.0000273	Pa×s	751.87	Joback Method
dvisc	0.0000157	Pa×s	834.49	Joback Method
dvisc	0.0000100	Pa×s	917.11	Joback Method
dvisc	0.0000069	Pa×s	999.72	Joback Method
dvisc	0.0000050	Pa×s	1082.34	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=U354359&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