Sebacic acid, 2-methoxyethyl tetradecyl ester

Inchi: InChI=1S/C27H52O5/c1-3-4-5-6-7-8-9-10-11-14-17-20-23-31-26(28)21-18-15-12-13-16-1
InchiKey: XSCPIHQSLZTLKF-UHFFFAOYSA-N
Formula: C27H52O5
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOC
Mol. weight [g/mol]: 456.70

Physical Properties

Property code	Value	Unit	Source
gf	-396.38	kJ/mol	Joback Method
hf	-1222.43	kJ/mol	Joback Method
hfus	72.45	kJ/mol	Joback Method
hvap	96.42	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.541		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	716.83	kPa	Joback Method
rinpol	3207.00		NIST Webbook
tb	992.16	K	Joback Method
tc	1231.88	K	Joback Method
tf	560.60	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.41	J/mol×K	992.16	Joback Method
cpg	1528.13	J/mol×K	1191.93	Joback Method
cpg	1514.93	J/mol×K	1151.98	Joback Method
cpg	1499.71	J/mol×K	1112.02	Joback Method
cpg	1482.41	J/mol×K	1072.07	Joback Method
cpg	1463.00	J/mol×K	1032.11	Joback Method
cpg	1539.36	J/mol×K	1231.88	Joback Method
dvisc	0.0000135	Pa×s	992.16	Joback Method
dvisc	0.0000181	Pa×s	920.23	Joback Method

dvisc	0.0000255	Pa×s	848.31	Joback Method
dvisc	0.0000383	Pa×s	776.38	Joback Method
dvisc	0.0000624	Pa×s	704.45	Joback Method
dvisc	0.0001135	Pa×s	632.53	Joback Method
dvisc	0.0002410	Pa×s	560.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355766&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
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