Sebacic acid, 2-ethoxyethyl pentadecyl ester

Inchi: InChI=1S/C29H56O5/c1-3-5-6-7-8-9-10-11-12-13-16-19-22-25-33-28(30)23-20-17-14-15
InchiKey: DVHRRGMPJAMEJQ-UHFFFAOYSA-N
Formula: C29H56O5
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOCC
Mol. weight [g/mol]: 484.75

Physical Properties

Property code	Value	Unit	Source
gf	-379.54	kJ/mol	Joback Method
hf	-1263.71	kJ/mol	Joback Method
hfus	77.63	kJ/mol	Joback Method
hvap	100.87	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	8.321		Crippen Method
mcvol	440.220	ml/mol	McGowan Method
pc	648.45	kPa	Joback Method
rinpol	3362.00		NIST Webbook
rinpol	3362.00		NIST Webbook
tb	1037.92	K	Joback Method
tc	1304.09	K	Joback Method
tf	583.14	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1570.74	J/mol×K	1037.92	Joback Method
cpg	1593.58	J/mol×K	1082.28	Joback Method
cpg	1613.69	J/mol×K	1126.64	Joback Method
cpg	1631.16	J/mol×K	1171.00	Joback Method
cpg	1646.07	J/mol×K	1215.37	Joback Method
cpg	1658.49	J/mol×K	1259.73	Joback Method
cpg	1668.51	J/mol×K	1304.09	Joback Method
dvisc	0.0001838	Pa×s	583.14	Joback Method

dvisc	0.0000851	Pa×s	658.94	Joback Method
dvisc	0.0000462	Pa×s	734.73	Joback Method
dvisc	0.0000281	Pa×s	810.53	Joback Method
dvisc	0.0000187	Pa×s	886.33	Joback Method
dvisc	0.0000132	Pa×s	962.12	Joback Method
dvisc	0.0000098	Pa×s	1037.92	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=U355641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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