

Sebacic acid, 2-ethoxyethyl tetradecyl ester

Inchi: InChI=1S/C28H54O5/c1-3-5-6-7-8-9-10-11-12-15-18-21-24-32-27(29)22-19-16-13-14-17
InchiKey: HYELWWIMULPUEY-UHFFFAOYSA-N
Formula: C28H54O5
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCCOCC
Mol. weight [g/mol]: 470.73

Physical Properties

Property code	Value	Unit	Source
gf	-387.96	kJ/mol	Joback Method
hf	-1243.07	kJ/mol	Joback Method
hfus	75.04	kJ/mol	Joback Method
hvap	98.64	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.931		Crippen Method
mcvol	426.130	ml/mol	McGowan Method
pc	681.36	kPa	Joback Method
rinsol	3258.00		NIST Webbook
tb	1015.04	K	Joback Method
tc	1267.21	K	Joback Method
tf	571.87	K	Joback Method
vc	1.669	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1505.96	J/molxK	1015.04	Joback Method
cpg	1528.16	J/molxK	1057.07	Joback Method
cpg	1547.93	J/molxK	1099.10	Joback Method
cpg	1565.34	J/molxK	1141.12	Joback Method
cpg	1580.45	J/molxK	1183.15	Joback Method
cpg	1593.32	J/molxK	1225.18	Joback Method
cpg	1604.01	J/molxK	1267.21	Joback Method
dvisc	0.0002107	Paxs	571.87	Joback Method
dvisc	0.0000984	Paxs	645.73	Joback Method

dvisc	0.0000537	Paxs	719.59	Joback Method
dvisc	0.0000329	Paxs	793.45	Joback Method
dvisc	0.0000218	Paxs	867.32	Joback Method
dvisc	0.0000155	Paxs	941.18	Joback Method
dvisc	0.0000115	Paxs	1015.04	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=U355640&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

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