

Sebacic acid, dodecyl 2-ethoxyethyl ester

Inchi:	InChI=1S/C26H50O5/c1-3-5-6-7-8-9-10-13-16-19-22-30-25(27)20-17-14-11-12-15-18-21
InchiKey:	SFNHDGZOKDDNQX-UHFFFAOYSA-N
Formula:	C26H50O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOCC
Mol. weight [g/mol]:	442.67

Physical Properties

Property code	Value	Unit	Source
gf	-404.80	kJ/mol	Joback Method
hf	-1201.79	kJ/mol	Joback Method
hfus	69.86	kJ/mol	Joback Method
hvap	94.19	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	7.151		Crippen Method
mvol	397.950	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	3061.00		NIST Webbook
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tb	969.28	K	Joback Method
tc	1198.00	K	Joback Method
tf	549.33	K	Joback Method
vc	1.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.16	J/molxK	969.28	Joback Method
cpg	1398.15	J/molxK	1007.40	Joback Method
cpg	1417.20	J/molxK	1045.52	Joback Method
cpg	1434.34	J/molxK	1083.64	Joback Method
cpg	1449.61	J/molxK	1121.76	Joback Method
cpg	1463.04	J/molxK	1159.88	Joback Method
cpg	1474.68	J/molxK	1198.00	Joback Method
dvisc	0.0002751	Paxs	549.33	Joback Method

dvisc	0.0001307	Paxs	619.32	Joback Method
dvisc	0.0000722	Paxs	689.31	Joback Method
dvisc	0.0000445	Paxs	759.31	Joback Method
dvisc	0.0000298	Paxs	829.30	Joback Method
dvisc	0.0000212	Paxs	899.29	Joback Method
dvisc	0.0000159	Paxs	969.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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