Sebacic acid, di(6-ethyloct-3-yl) ester

Inchi: InChI=1S/C30H58O4/c1-7-25(8-2)21-23-27(11-5)33-29(31)19-17-15-13-14-16-18-20-30(
InchiKey: QVEPSOOXKQRECX-UHFFFAOYSA-N
Formula: C30H58O4
SMILES: CCC(CC)CCC(CC)OC(=O)CCCCCCCCC(=O)OC(CC)CCC(CC)CC
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-275.88	kJ/mol	Joback Method
hf	-1173.25	kJ/mol	Joback Method
hfus	64.94	kJ/mol	Joback Method
hvap	99.13	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	9.184		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	633.20	kPa	Joback Method
rinpol	3097.00		NIST Webbook
rinpol	3097.00		NIST Webbook
tb	1036.62	K	Joback Method
tc	1290.93	K	Joback Method
tf	512.18	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1606.02	J/mol×K	1036.62	Joback Method
cpg	1628.91	J/mol×K	1079.01	Joback Method
cpg	1649.42	J/mol×K	1121.39	Joback Method
cpg	1667.65	J/mol×K	1163.78	Joback Method
cpg	1683.71	J/mol×K	1206.16	Joback Method
cpg	1697.67	J/mol×K	1248.55	Joback Method
cpg	1709.66	J/mol×K	1290.93	Joback Method
dvisc	0.0004148	Pa×s	512.18	Joback Method

dvisc	0.0001320	Pa×s	599.59	Joback Method
dvisc	0.0000562	Pa×s	686.99	Joback Method
dvisc	0.0000290	Pa×s	774.40	Joback Method
dvisc	0.0000171	Pa×s	861.81	Joback Method
dvisc	0.0000111	Pa×s	949.21	Joback Method
dvisc	0.0000078	Pa×s	1036.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354195&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