Di 2-ethyl hexyl 2-ethyl suberate

Inchi: InChI=1S/C26H50O4/c1-6-11-16-22(8-3)20-29-25(27)19-15-13-14-18-24(10-5)26(28)30-
InchiKey: XNLFDVGJJPYNGF-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCC(CC)COC(=O)CCCCCC(CC)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 426.67
CAS: 922-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-307.12	kJ/mol	Joback Method
hf	-1085.41	kJ/mol	Joback Method
hfus	58.10	kJ/mol	Joback Method
hvap	90.62	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	7.482		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	772.46	kPa	Joback Method
tb	945.54	K	Joback Method
tc	1161.05	K	Joback Method
tf	482.10	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.32	J/mol×K	945.54	Joback Method
cpg	1434.66	J/mol×K	1125.13	Joback Method
cpg	1420.12	J/mol×K	1089.21	Joback Method
cpg	1404.07	J/mol×K	1053.29	Joback Method
cpg	1386.45	J/mol×K	1017.38	Joback Method
cpg	1367.21	J/mol×K	981.46	Joback Method
cpg	1447.72	J/mol×K	1161.05	Joback Method
dvisc	0.0000164	Pa×s	945.54	Joback Method
dvisc	0.0000230	Pa×s	868.30	Joback Method

dvisc	0.0000345	Pa×s	791.06	Joback Method
dvisc	0.0000565	Pa×s	713.82	Joback Method
dvisc	0.0001044	Pa×s	636.58	Joback Method
dvisc	0.0002284	Pa×s	559.34	Joback Method
dvisc	0.0006421	Pa×s	482.10	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C922098&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume