Mono-2-ethyl hexyl sebacate

Inchi: InChI=1S/C18H34O4/c1-3-5-10-13-16(4-2)22-18(21)15-12-9-7-6-8-11-14-17(19)20/h16H
InchiKey: JGQWKLHHTRIVSL-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCC(CC)OC(=O)CCCCCCCCC(=O)O
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-401.42	kJ/mol	Joback Method
hf	-929.74	kJ/mol	Joback Method
hfus	47.33	kJ/mol	Joback Method
hvap	87.85	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.094		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
tb	833.14	K	Joback Method
tc	1020.80	K	Joback Method
tf	460.53	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.30	J/mol×K	833.14	Joback Method
cpg	905.22	J/mol×K	864.42	Joback Method
cpg	920.20	J/mol×K	895.69	Joback Method
cpg	934.27	J/mol×K	926.97	Joback Method
cpg	947.45	J/mol×K	958.24	Joback Method
cpg	959.77	J/mol×K	989.52	Joback Method
cpg	971.26	J/mol×K	1020.80	Joback Method
dvisc	0.0009805	Pa×s	460.53	Joback Method
dvisc	0.0003169	Pa×s	522.63	Joback Method
dvisc	0.0001302	Pa×s	584.73	Joback Method

dvisc	0.0000635	Pa×s	646.84	Joback Method
dvisc	0.0000351	Pa×s	708.94	Joback Method
dvisc	0.0000213	Pa×s	771.04	Joback Method
dvisc	0.0000140	Pa×s	833.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000977&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

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