2-ethylhexyl 2-ethylhexanoate

Inchi: InChI=1S/C16H32O2/c1-5-9-11-14(7-3)13-18-16(17)15(8-4)12-10-6-2/h14-15H,5-13H2,1
InchiKey: OUCGJMIVSYHBEC-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCC(CC)COC(=O)C(CC)CCCC
Mol. weight [g/mol]: 256.43
CAS: 7425-14-1

Physical Properties

Property code	Value	Unit	Source
af	0.7258		Cheméo Relay (1.0)
hf	-696.68	kJ/mol	Cheméo Relay (1.0)
hfus	32.94	kJ/mol	Joback Method
hvap	74.47	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.11		Cheméo Relay (1.0)
logp	4.962		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
tb	538.92	K	Cheméo Relay (1.0)
tc	726.02	K	Cheméo Relay (1.0)
tf	193.11	K	Cheméo Relay (1.0)
vc	0.895	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.61	J/mol×K	640.89	Joback Method
cpg	695.06	J/mol×K	669.55	Joback Method
cpg	712.71	J/mol×K	698.21	Joback Method
cpg	729.56	J/mol×K	726.87	Joback Method
cpg	745.63	J/mol×K	755.53	Joback Method
cpg	760.94	J/mol×K	784.19	Joback Method
cpg	775.50	J/mol×K	812.85	Joback Method
dvisc	0.0043257	Pa×s	312.24	Joback Method
dvisc	0.0014680	Pa×s	367.01	Joback Method

dvisc	0.0006596	Pa×s	421.79	Joback Method
dvisc	0.0003562	Pa×s	476.56	Joback Method
dvisc	0.0002184	Pa×s	531.34	Joback Method
dvisc	0.0001468	Pa×s	586.12	Joback Method
dvisc	0.0001055	Pa×s	640.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49106e+01
Coeff. B	-4.87568e+03
Coeff. C	-9.90960e+01
Temperature range (K), min.	432.52
Temperature range (K), max.	607.02

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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