2-methylheptyl propanoate

Inchi: InChI=1S/C11H22O2/c1-4-6-7-8-10(3)9-13-11(12)5-2/h10H,4-9H2,1-3H3
InchiKey: USOFNPBSEVMXHD-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCCCCC(C)COC(=O)CC
Mol. weight [g/mol]: 186.29
CAS: ---

Physical Properties

Property code	Value	Unit	Source
gf	-194.62	kJ/mol	Joback Method
hf	-520.45	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.156		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
tb	526.93	K	Joback Method
tc	701.19	K	Joback Method
tf	270.89	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.48	J/mol×K	526.93	Joback Method
cpg	430.78	J/mol×K	555.97	Joback Method
cpg	445.49	J/mol×K	585.02	Joback Method
cpg	459.60	J/mol×K	614.06	Joback Method
cpg	473.13	J/mol×K	643.11	Joback Method
cpg	486.09	J/mol×K	672.15	Joback Method
cpg	498.48	J/mol×K	701.19	Joback Method

dvisc	0.0044896	Pa×s	270.89	Joback Method
dvisc	0.0018616	Pa×s	313.56	Joback Method
dvisc	0.0009531	Pa×s	356.24	Joback Method
dvisc	0.0005632	Pa×s	398.91	Joback Method
dvisc	0.0003684	Pa×s	441.58	Joback Method
dvisc	0.0002597	Pa×s	484.26	Joback Method
dvisc	0.0001937	Pa×s	526.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48133e+01
Coeff. B	-4.24799e+03
Coeff. C	-7.72730e+01
Temperature range (K), min.	369.72
Temperature range (K), max.	524.35

Sources

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=R222830&Units=SI

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

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

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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume