2-heptyl octanoate

Other names: 1-Methylhexyl octanoate
Inchi: InChI=1S/C15H30O2/c1-4-6-8-9-11-13-15(16)17-14(3)12-10-7-5-2/h14H,4-13H2,1-3H3
InchiKey: UKPOONOGHLYURR-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCCCCCCC(=O)OC(C)CCCCC
Mol. weight [g/mol]: 242.40
CAS: 55193-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-160.94	kJ/mol	Joback Method
hf	-603.01	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.859		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
ripol	1772.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1788.00		NIST Webbook
tb	618.45	K	Joback Method
tc	788.43	K	Joback Method
tf	315.97	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.09	J/mol×K	618.45	Joback Method
cpg	638.80	J/mol×K	646.78	Joback Method
cpg	655.75	J/mol×K	675.11	Joback Method
cpg	671.98	J/mol×K	703.44	Joback Method
cpg	687.48	J/mol×K	731.77	Joback Method

cpg	702.28	J/mol×K	760.10	Joback Method
cpg	716.38	J/mol×K	788.43	Joback Method
dvisc	0.0034492	Pa×s	315.97	Joback Method
dvisc	0.0013649	Pa×s	366.38	Joback Method
dvisc	0.0006759	Pa×s	416.80	Joback Method
dvisc	0.0003895	Pa×s	467.21	Joback Method
dvisc	0.0002499	Pa×s	517.62	Joback Method
dvisc	0.0001735	Pa×s	568.04	Joback Method
dvisc	0.0001278	Pa×s	618.45	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55193323&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume