Decanoic acid, pentyl ester

Other names: Pentyl decanoate
Inchi: InChI=1S/C15H30O2/c1-3-5-7-8-9-10-11-13-15(16)17-14-12-6-4-2/h3-14H2,1-2H3
InchiKey: BGYFCELTJPRWBA-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 242.40
CAS: 5933-87-9

Physical Properties

Property code	Value	Unit	Source
gf	-158.50	kJ/mol	Joback Method
hf	-597.73	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.861		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	618.89	K	Joback Method
tc	786.41	K	Joback Method
tf	330.97	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.74	J/mol×K	618.89	Joback Method
cpg	700.70	J/mol×K	758.49	Joback Method
cpg	686.10	J/mol×K	730.57	Joback Method
cpg	670.81	J/mol×K	702.65	Joback Method
cpg	654.83	J/mol×K	674.73	Joback Method

cpg	638.14	J/mol×K	646.81	Joback Method
cpg	714.65	J/mol×K	786.41	Joback Method
dvisc	0.0001371	Pa×s	618.89	Joback Method
dvisc	0.0001822	Pa×s	570.90	Joback Method
dvisc	0.0002549	Pa×s	522.92	Joback Method
dvisc	0.0003819	Pa×s	474.93	Joback Method
dvisc	0.0006264	Pa×s	426.94	Joback Method
dvisc	0.0011647	Pa×s	378.96	Joback Method
dvisc	0.0025922	Pa×s	330.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5933879&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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