Pentyl oleate

Inchi: InChI=1S/C23H44O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-23(24)25-22-20-6
InchiKey: YEUKJHYLBPPSQJ-SEYXRHQNSA-N
Formula: C23H44O2
SMILES: CCCCCCCC/C=C\CCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 352.60

Physical Properties

Property code	Value	Unit	Source
af	1.0003		Cheméo Relay (1.0)
gf	-10.92	kJ/mol	Joback Method
hf	-753.04	kJ/mol	Cheméo Relay (1.0)
hfus	58.31	kJ/mol	Joback Method
hvap	110.01	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
log10ws	-7.18		Cheméo Relay (1.0)
logp	7.757		Crippen Method
mcvol	338.070	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	2421.70		NIST Webbook
rinpol	2421.70		NIST Webbook
tb	610.05	K	Cheméo Relay (1.0)
tc	802.76	K	Cheméo Relay (1.0)
tf	260.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.83	J/mol×K	806.09	Joback Method
cpg	1089.32	J/mol×K	836.45	Joback Method
cpg	1108.77	J/mol×K	866.81	Joback Method
cpg	1127.22	J/mol×K	897.16	Joback Method
cpg	1144.72	J/mol×K	927.52	Joback Method
cpg	1161.30	J/mol×K	957.88	Joback Method
cpg	1177.00	J/mol×K	988.24	Joback Method

dvisc	0.0011170	Pa×s	416.05	Joback Method
dvisc	0.0004469	Pa×s	481.06	Joback Method
dvisc	0.0002224	Pa×s	546.06	Joback Method
dvisc	0.0001283	Pa×s	611.07	Joback Method
dvisc	0.0000823	Pa×s	676.08	Joback Method
dvisc	0.0000571	Pa×s	741.08	Joback Method
dvisc	0.0000420	Pa×s	806.09	Joback Method

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142574&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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