ETHYL ALPHA-PENTYLACETOACETATE

Other names: Ethyl 2-acetylheptanoate
Inchi: InChI=1S/C11H20O3/c1-4-6-7-8-10(9(3)12)11(13)14-5-2/h10H,4-8H2,1-3H3
InchiKey: XIGZBCUFFUBWDM-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CCCCCC(C(C)=O)C(=O)OCC
Mol. weight [g/mol]: 200.28

Physical Properties

Property code	Value	Unit	Source
af	0.5881		Cheméo Relay (1.0)
hf	-708.46	kJ/mol	Cheméo Relay (1.0)
hfus	25.11	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.26		Cheméo Relay (1.0)
logp	2.335		Crippen Method
mcvol	174.860	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
tb	509.39	K	Cheméo Relay (1.0)
tc	689.18	K	Cheméo Relay (1.0)
tf	259.10	K	Cheméo Relay (1.0)
vc	0.631	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.02	J/mol×K	580.80	Joback Method
cpg	515.97	J/mol×K	763.33	Joback Method
cpg	504.69	J/mol×K	732.91	Joback Method
cpg	492.80	J/mol×K	702.49	Joback Method
cpg	480.30	J/mol×K	672.07	Joback Method
cpg	467.17	J/mol×K	641.64	Joback Method
cpg	453.42	J/mol×K	611.22	Joback Method
dvisc	0.0005420	Pa×s	450.81	Joback Method
dvisc	0.0002010	Pa×s	580.80	Joback Method

dvisc	0.0002652	Pa×s	537.47	Joback Method
dvisc	0.0003675	Pa×s	494.14	Joback Method
dvisc	0.0032667	Pa×s	320.82	Joback Method
dvisc	0.0008685	Pa×s	407.48	Joback Method
dvisc	0.0015567	Pa×s	364.15	Joback Method

Sources

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=C24317940&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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