ETHYL 3-METHYLDECANOATE

Inchi: InChI=1S/C13H26O2/c1-4-6-7-8-9-10-12(3)11-13(14)15-5-2/h12H,4-11H2,1-3H3
InchiKey: FSCWTVVABUSMIQ-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCCCCC(C)CC(=O)OCC
Mol. weight [g/mol]: 214.35

Physical Properties

Property code	Value	Unit	Source
af	0.6622		Cheméo Relay (1.0)
gf	-177.78	kJ/mol	Joback Method
hf	-641.88	kJ/mol	Cheméo Relay (1.0)
hfus	28.69	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-4.43		Cheméo Relay (1.0)
logp	3.936		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
ripol	1571.00		NIST Webbook
ripol	1571.00		NIST Webbook
tb	494.32	K	Cheméo Relay (1.0)
tc	684.97	K	Cheméo Relay (1.0)
tf	220.78	K	Cheméo Relay (1.0)
vc	0.752	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.10	J/mol×K	572.69	Joback Method
cpg	531.74	J/mol×K	601.30	Joback Method
cpg	547.70	J/mol×K	629.91	Joback Method
cpg	563.00	J/mol×K	658.53	Joback Method
cpg	577.64	J/mol×K	687.14	Joback Method
cpg	591.64	J/mol×K	715.75	Joback Method

cpg	605.00	J/mol×K	744.36	Joback Method
dvisc	0.0040106	Pa×s	293.43	Joback Method
dvisc	0.0016218	Pa×s	339.97	Joback Method
dvisc	0.0008156	Pa×s	386.52	Joback Method
dvisc	0.0004755	Pa×s	433.06	Joback Method
dvisc	0.0003078	Pa×s	479.60	Joback Method
dvisc	0.0002152	Pa×s	526.15	Joback Method
dvisc	0.0001594	Pa×s	572.69	Joback Method

Sources

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=C73105701&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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