

Hexanoic acid, 2-ethyl-, ethyl ester

Other names:	Ethyl 2-ethylcaproate Ethyl 2-ethylhexanoate Ethyl«alpha»-ethylhexanoate EthylÂ«alphaÂ»-ethylhexanoate
Inchi:	InChI=1S/C10H20O2/c1-4-7-8-9(5-2)10(11)12-6-3/h9H,4-8H2,1-3H3
InchiKey:	YXAGIRHBJJLWHW-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCC(CC)C(=O)OCC
Mol. weight [g/mol]:	172.26
CAS:	2983-37-1

Physical Properties

Property code	Value	Unit	Source
gf	-203.04	kJ/mol	Joback Method
hf	-499.81	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.766		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1107.00		NIST Webbook
tb	504.05	K	Joback Method
tc	679.81	K	Joback Method
tf	259.62	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.31	J/molxK	504.05	Joback Method
cpg	382.82	J/molxK	533.34	Joback Method

cpg	396.77	J/mol×K	562.64	Joback Method
cpg	410.17	J/mol×K	591.93	Joback Method
cpg	423.03	J/mol×K	621.22	Joback Method
cpg	435.35	J/mol×K	650.52	Joback Method
cpg	447.14	J/mol×K	679.81	Joback Method
dvisc	0.0046674	Paxs	259.62	Joback Method
dvisc	0.0019627	Paxs	300.36	Joback Method
dvisc	0.0010151	Paxs	341.10	Joback Method
dvisc	0.0006043	Paxs	381.84	Joback Method
dvisc	0.0003976	Paxs	422.57	Joback Method
dvisc	0.0002816	Paxs	463.31	Joback Method
dvisc	0.0002109	Paxs	504.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49788e+01
Coeff. B	-4.17429e+03
Coeff. C	-7.28470e+01
Temperature range (K), min.	356.98
Temperature range (K), max.	504.64

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2983371&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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