

Ethyl hydrogen suberate

Inchi:	InChI=1S/C10H18O4/c1-2-14-10(13)8-6-4-3-5-7-9(11)12/h2-8H2,1H3,(H,11,12)
InchiKey:	KCFVQEAPUOVXTH-UHFFFAOYSA-N
Formula:	C10H18O4
SMILES:	CCOC(=O)CCCCCCC(=O)O
Mol. weight [g/mol]:	202.25

Physical Properties

Property code	Value	Unit	Source
gf	-466.34	kJ/mol	Joback Method
hf	-759.34	kJ/mol	Joback Method
hfus	30.13	kJ/mol	Joback Method
hvap	70.44	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.975		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1553.00		NIST Webbook
tb	650.54	K	Joback Method
tc	825.37	K	Joback Method
tf	385.37	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.48	J/mol×K	650.54	Joback Method
cpg	457.93	J/mol×K	679.68	Joback Method
cpg	468.85	J/mol×K	708.82	Joback Method
cpg	479.25	J/mol×K	737.96	Joback Method
cpg	489.14	J/mol×K	767.09	Joback Method
cpg	498.52	J/mol×K	796.23	Joback Method
cpg	507.39	J/mol×K	825.37	Joback Method
dvisc	0.0029033	Pa×s	385.37	Joback Method
dvisc	0.0011146	Pa×s	429.56	Joback Method

dvisc	0.0005116	Pa×s	473.76	Joback Method
dvisc	0.0002682	Pa×s	517.95	Joback Method
dvisc	0.0001556	Pa×s	562.15	Joback Method
dvisc	0.0000977	Pa×s	606.35	Joback Method
dvisc	0.0000654	Pa×s	650.54	Joback Method

Sources

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=U375801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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