Octanedioic acid, 2-ethyl-

Other names: 2-Ethylsuberic acid
2-ethyloctanedioic acid
Inchi: InChI=1S/C10H18O4/c1-2-8(10(13)14)6-4-3-5-7-9(11)12/h8H,2-7H2,1H3,(H,11,12)(H,13
InchiKey: WUDDSDIHJHPJRP-UHFFFAOYSA-N
Formula: C10H18O4
SMILES: CCC(CCCCCC(=O)O)C(=O)O
Mol. weight [g/mol]: 202.25
CAS: 3971-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-500.60	kJ/mol	Joback Method
hf	-784.63	kJ/mol	Joback Method
hfus	29.51	kJ/mol	Joback Method
hvap	84.32	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.132		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	719.86	K	Joback Method
tc	895.66	K	Joback Method
tf	408.96	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.16	J/mol×K	719.86	Joback Method
cpg	484.26	J/mol×K	749.16	Joback Method
cpg	493.84	J/mol×K	778.46	Joback Method
cpg	502.91	J/mol×K	807.76	Joback Method
cpg	511.50	J/mol×K	837.06	Joback Method
cpg	519.62	J/mol×K	866.36	Joback Method
cpg	527.29	J/mol×K	895.66	Joback Method

dvisc	0.0034654	Pa×s	408.96	Joback Method
dvisc	0.0008245	Pa×s	460.78	Joback Method
dvisc	0.0002622	Pa×s	512.59	Joback Method
dvisc	0.0001029	Pa×s	564.41	Joback Method
dvisc	0.0000473	Pa×s	616.23	Joback Method
dvisc	0.0000245	Pa×s	668.04	Joback Method
dvisc	0.0000140	Pa×s	719.86	Joback Method

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=C3971333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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