Heptanoic acid, 2,5-diethyl-

Other names: 2,5-Diethylheptanoic acid
Inchi: InChI=1S/C11H22O2/c1-4-9(5-2)7-8-10(6-3)11(12)13/h9-10H,4-8H2,1-3H3,(H,12,13)
InchiKey: XQWMZYYVMUUGRU-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCC(CC)CCC(CC)C(=O)O
Mol. weight [g/mol]: 186.29
CAS: 54774-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-228.88	kJ/mol	Joback Method
hf	-545.74	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.314		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
ripol	2001.00		NIST Webbook
ripol	2001.00		NIST Webbook
tb	596.25	K	Joback Method
tc	767.88	K	Joback Method
tf	294.48	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.78	J/mol×K	596.25	Joback Method
cpg	466.41	J/mol×K	624.86	Joback Method
cpg	479.44	J/mol×K	653.46	Joback Method
cpg	491.88	J/mol×K	682.07	Joback Method
cpg	503.75	J/mol×K	710.67	Joback Method
cpg	515.07	J/mol×K	739.28	Joback Method

cpg	525.85	J/mol×K	767.88	Joback Method
dvisc	0.0258374	Pa×s	294.48	Joback Method
dvisc	0.0048244	Pa×s	344.78	Joback Method
dvisc	0.0013810	Pa×s	395.07	Joback Method
dvisc	0.0005244	Pa×s	445.37	Joback Method
dvisc	0.0002424	Pa×s	495.66	Joback Method
dvisc	0.0001291	Pa×s	545.95	Joback Method
dvisc	0.0000765	Pa×s	596.25	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=C54774844&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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