

n-Capric acid n-heptyl ester

Other names:	Decanoic acid, heptyl ester Heptyl decanoate
Inchi:	InChI=1S/C17H34O2/c1-3-5-7-9-10-11-13-15-17(18)19-16-14-12-8-6-4-2/h3-16H2,1-2H3
InchiKey:	MPLLSYWBBPPERF-UHFFFAOYSA-N
Formula:	C17H34O2
SMILES:	CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	270.45
CAS:	60160-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-141.66	kJ/mol	Joback Method
hf	-639.01	kJ/mol	Joback Method
hfus	42.57	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.641		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1878.00		NIST Webbook
rinpol	1885.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1864.00		NIST Webbook
tb	664.65	K	Joback Method
tc	832.26	K	Joback Method
tf	353.51	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.28	J/mol×K	664.65	Joback Method
cpg	816.25	J/mol×K	804.33	Joback Method
cpg	800.97	J/mol×K	776.39	Joback Method

cpg	784.95	J/molxK	748.46	Joback Method
cpg	768.17	J/molxK	720.52	Joback Method
cpg	750.62	J/molxK	692.59	Joback Method
cpg	830.80	J/molxK	832.26	Joback Method
dvisc	0.0001081	Paxs	664.65	Joback Method
dvisc	0.0001445	Paxs	612.79	Joback Method
dvisc	0.0002038	Paxs	560.94	Joback Method
dvisc	0.0003083	Paxs	509.08	Joback Method
dvisc	0.0005124	Paxs	457.22	Joback Method
dvisc	0.0009695	Paxs	405.37	Joback Method
dvisc	0.0022120	Paxs	353.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60160170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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