

Octanoic acid, 2-octyl ester

Other names:	sec-octyl octanoate
Inchi:	InChI=1S/C16H32O2/c1-4-6-8-10-12-14-16(17)18-15(3)13-11-9-7-5-2/h15H,4-14H2,1-3H
InchiKey:	RUYSQUUOTCIKAT-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCC(=O)OC(C)CCCCC
Mol. weight [g/mol]:	256.42
CAS:	55193-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-152.52	kJ/mol	Joback Method
hf	-623.65	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.249		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
tb	641.33	K	Joback Method
tc	810.93	K	Joback Method
tf	327.24	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.23	J/molxK	641.33	Joback Method
cpg	694.40	J/molxK	669.60	Joback Method
cpg	711.78	J/molxK	697.86	Joback Method
cpg	728.40	J/molxK	726.13	Joback Method
cpg	744.26	J/molxK	754.40	Joback Method
cpg	759.39	J/molxK	782.67	Joback Method
cpg	773.80	J/molxK	810.93	Joback Method
dvisc	0.0031617	Paxs	327.24	Joback Method

dvisc	0.0012389	Paxs	379.59	Joback Method
dvisc	0.0006092	Paxs	431.94	Joback Method
dvisc	0.0003493	Paxs	484.28	Joback Method
dvisc	0.0002232	Paxs	536.63	Joback Method
dvisc	0.0001544	Paxs	588.98	Joback Method
dvisc	0.0001135	Paxs	641.33	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=C55193334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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