

9-Octadecenoic acid, butyl ester

Inchi:	InChI=1S/C22H42O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22(23)24-21-6-4-2
InchiKey:	WIBFFTLQMKKBLZ-UHFFFAOYSA-N
Formula:	C22H42O2
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	338.57
CAS:	13171-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-19.34	kJ/mol	Joback Method
hf	-624.99	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.367		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
tb	783.21	K	Joback Method
tc	962.10	K	Joback Method
tf	404.78	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.83	J/molxK	783.21	Joback Method
cpg	1026.84	J/molxK	813.03	Joback Method
cpg	1045.86	J/molxK	842.84	Joback Method
cpg	1063.93	J/molxK	872.66	Joback Method
cpg	1081.08	J/molxK	902.47	Joback Method
cpg	1097.36	J/molxK	932.29	Joback Method
cpg	1112.80	J/molxK	962.10	Joback Method
dvisc	0.0012526	Paxs	404.78	Joback Method
dvisc	0.0005052	Paxs	467.85	Joback Method

dvisc	0.0002528	Paxs	530.92	Joback Method
dvisc	0.0001465	Paxs	593.99	Joback Method
dvisc	0.0000943	Paxs	657.07	Joback Method
dvisc	0.0000656	Paxs	720.14	Joback Method
dvisc	0.0000483	Paxs	783.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13171249&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
mccvol:	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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