

Valeric acid, hexadecyl ester

Inchi:	InChI=1S/C21H42O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-23-21(22)19-6-4-2/h3
InchiKey:	OSIFZWLCMRYWEE-UHFFFAOYSA-N
Formula:	C21H42O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC
Mol. weight [g/mol]:	326.56
CAS:	125164-54-7

Physical Properties

Property code	Value	Unit	Source
gf	-107.98	kJ/mol	Joback Method
hf	-721.57	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.201		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
tb	756.17	K	Joback Method
tc	929.77	K	Joback Method
tf	398.59	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.32	J/molxK	756.17	Joback Method
cpg	1060.46	J/molxK	900.83	Joback Method
cpg	1044.06	J/molxK	871.90	Joback Method
cpg	1026.77	J/molxK	842.97	Joback Method
cpg	1008.57	J/molxK	814.04	Joback Method
cpg	989.43	J/molxK	785.10	Joback Method
cpg	1075.99	J/molxK	929.77	Joback Method
dvisc	0.0000640	Paxs	756.17	Joback Method
dvisc	0.0000864	Paxs	696.57	Joback Method

dvisc	0.0001235	Paxs	636.98	Joback Method
dvisc	0.0001899	Paxs	577.38	Joback Method
dvisc	0.0003224	Paxs	517.78	Joback Method
dvisc	0.0006283	Paxs	458.19	Joback Method
dvisc	0.0014949	Paxs	398.59	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=C125164547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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