

4-Pentenoic acid, 2-methyl-, heptadecyl ester

Inchi: InChI=1S/C23H44O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-25-23(24)22(3)20
InchiKey: BQNQFBBQCNZZGY-UHFFFAOYSA-N
Formula: C23H44O2
SMILES: C=CCC(C)C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 352.59

Physical Properties

Property code	Value	Unit	Source
gf	-5.74	kJ/mol	Joback Method
hf	-642.70	kJ/mol	Joback Method
hfus	53.31	kJ/mol	Joback Method
hvap	74.89	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	7.613		Crippen Method
mcvol	338.070	ml/mol	McGowan Method
pc	901.80	kPa	Joback Method
rinpola	2414.00		NIST Webbook
rinpola	2414.00		NIST Webbook
tb	798.17	K	Joback Method
tc	978.88	K	Joback Method
tf	404.37	K	Joback Method
vc	1.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.85	J/molxK	798.17	Joback Method
cpg	1159.46	J/molxK	948.76	Joback Method
cpg	1142.93	J/molxK	918.64	Joback Method
cpg	1125.44	J/molxK	888.52	Joback Method
cpg	1106.95	J/molxK	858.41	Joback Method
cpg	1087.44	J/molxK	828.29	Joback Method
cpg	1175.06	J/molxK	978.88	Joback Method
dvisc	0.0000473	Paxs	798.17	Joback Method

dvisc	0.0000649	Paxs	732.54	Joback Method
dvisc	0.0000948	Paxs	666.90	Joback Method
dvisc	0.0001504	Paxs	601.27	Joback Method
dvisc	0.0002670	Paxs	535.64	Joback Method
dvisc	0.0005564	Paxs	470.00	Joback Method
dvisc	0.0014720	Paxs	404.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406120&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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