2-Heptenoic acid, pentadecyl ester

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

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
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
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/mol×K	783.21	Joback Method
cpg	1026.84	J/mol×K	813.03	Joback Method
cpg	1045.86	J/mol×K	842.84	Joback Method
cpg	1063.93	J/mol×K	872.66	Joback Method
cpg	1081.08	J/mol×K	902.47	Joback Method
cpg	1097.36	J/mol×K	932.29	Joback Method
cpg	1112.80	J/mol×K	962.10	Joback Method
dvisc	0.0012526	Pa×s	404.78	Joback Method

dvisc	0.0005052	Pa×s	467.85	Joback Method
dvisc	0.0002528	Pa×s	530.92	Joback Method
dvisc	0.0001465	Pa×s	593.99	Joback Method
dvisc	0.0000943	Pa×s	657.07	Joback Method
dvisc	0.0000656	Pa×s	720.14	Joback Method
dvisc	0.0000483	Pa×s	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=U406100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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