

4-Ethylbenzoic acid, pentadecyl ester

Inchi:	InChI=1S/C24H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-21-26-24(25)23-19-17-22(4-2)
InchiKey:	UVXACWOBZLNVOG-UHFFFAOYSA-N
Formula:	C24H40O2
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	360.57

Physical Properties

Property code	Value	Unit	Source
gf	20.06	kJ/mol	Joback Method
hf	-558.43	kJ/mol	Joback Method
hfus	54.35	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	7.497		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
rinpol	2676.60		NIST Webbook
tb	856.47	K	Joback Method
tc	1052.40	K	Joback Method
tf	471.34	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.56	J/molxK	856.47	Joback Method
cpg	1152.27	J/molxK	1019.75	Joback Method
cpg	1137.51	J/molxK	987.09	Joback Method
cpg	1121.70	J/molxK	954.44	Joback Method
cpg	1104.80	J/molxK	921.78	Joback Method
cpg	1086.77	J/molxK	889.13	Joback Method
cpg	1166.02	J/molxK	1052.40	Joback Method
dvisc	0.0000433	Paxs	856.47	Joback Method
dvisc	0.0000571	Paxs	792.28	Joback Method

dvisc	0.0000790	Paxs	728.09	Joback Method
dvisc	0.0001165	Paxs	663.90	Joback Method
dvisc	0.0001865	Paxs	599.72	Joback Method
dvisc	0.0003343	Paxs	535.53	Joback Method
dvisc	0.0007027	Paxs	471.34	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292349&Units=SI

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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