4-Ethylbenzoic acid, hexadecyl ester

Inchi: InChI=1S/C25H42O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-27-25(26)24-20-18-23
InchiKey: DONBQABLRPKJKA-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 374.60

Physical Properties

Property code	Value	Unit	Source
gf	28.48	kJ/mol	Joback Method
hf	-579.07	kJ/mol	Joback Method
hfus	56.94	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	7.887		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2757.50		NIST Webbook
tb	879.35	K	Joback Method
tc	1078.25	K	Joback Method
tf	482.61	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.80	J/mol×K	879.35	Joback Method
cpg	1215.57	J/mol×K	1045.10	Joback Method
cpg	1200.69	J/mol×K	1011.95	Joback Method
cpg	1184.71	J/mol×K	978.80	Joback Method
cpg	1167.61	J/mol×K	945.65	Joback Method
cpg	1149.32	J/mol×K	912.50	Joback Method
cpg	1229.43	J/mol×K	1078.25	Joback Method
dvisc	0.0000376	Pa×s	879.35	Joback Method
dvisc	0.0000496	Pa×s	813.23	Joback Method

dvisc	0.0000689	Pa×s	747.10	Joback Method
dvisc	0.0001020	Pa×s	680.98	Joback Method
dvisc	0.0001641	Pa×s	614.86	Joback Method
dvisc	0.0002964	Pa×s	548.73	Joback Method
dvisc	0.0006292	Pa×s	482.61	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=U292350&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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