4-Ethylbenzoic acid, 4-hexadecyl ester

Inchi: InChI=1S/C25H42O2/c1-4-7-8-9-10-11-12-13-14-15-17-24(16-5-2)27-25(26)23-20-18-22
InchiKey: JLUAINKQSUGVNL-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCCC(CCC)OC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 374.60

Physical Properties

Property code	Value	Unit	Source
gf	26.04	kJ/mol	Joback Method
hf	-584.35	kJ/mol	Joback Method
hfus	53.42	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	7.886		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	947.91	kPa	Joback Method
rinpol	2604.70		NIST Webbook
rinpol	2604.70		NIST Webbook
tb	878.91	K	Joback Method
tc	1078.47	K	Joback Method
tf	467.61	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.24	J/mol×K	878.91	Joback Method
cpg	1216.06	J/mol×K	1045.21	Joback Method
cpg	1201.20	J/mol×K	1011.95	Joback Method
cpg	1185.24	J/mol×K	978.69	Joback Method
cpg	1168.12	J/mol×K	945.43	Joback Method
cpg	1149.81	J/mol×K	912.17	Joback Method
cpg	1229.87	J/mol×K	1078.47	Joback Method
dvisc	0.0000344	Pa×s	878.91	Joback Method

dvisc	0.0000461	Pa×s	810.36	Joback Method
dvisc	0.0000653	Pa×s	741.81	Joback Method
dvisc	0.0000992	Pa×s	673.26	Joback Method
dvisc	0.0001659	Pa×s	604.71	Joback Method
dvisc	0.0003164	Pa×s	536.16	Joback Method
dvisc	0.0007290	Pa×s	467.61	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292203&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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