

4-Ethylbenzoic acid, octadecyl ester

Inchi: InChI=1S/C27H46O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-29-27(28)26-22
InchiKey: INTMIYCHAIDNOI-UHFFFAOYSA-N
Formula: C27H46O2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 402.65

Physical Properties

Property code	Value	Unit	Source
gf	45.32	kJ/mol	Joback Method
hf	-620.35	kJ/mol	Joback Method
hfus	62.12	kJ/mol	Joback Method
hvap	87.79	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	8.667		Crippen Method
mcvol	374.970	ml/mol	McGowan Method
pc	841.13	kPa	Joback Method
rinpol	2957.70		NIST Webbook
tb	925.11	K	Joback Method
tc	1132.60	K	Joback Method
tf	505.15	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.10	J/molxK	925.11	Joback Method
cpg	1276.35	J/molxK	959.69	Joback Method
cpg	1295.24	J/molxK	994.27	Joback Method
cpg	1312.83	J/molxK	1028.86	Joback Method
cpg	1329.18	J/molxK	1063.44	Joback Method
cpg	1344.35	J/molxK	1098.02	Joback Method
cpg	1358.41	J/molxK	1132.60	Joback Method
dvisc	0.0004990	Paxs	505.15	Joback Method
dvisc	0.0002307	Paxs	575.14	Joback Method

dvisc	0.0001261	Paxs	645.14	Joback Method
dvisc	0.0000775	Paxs	715.13	Joback Method
dvisc	0.0000520	Paxs	785.12	Joback Method
dvisc	0.0000372	Paxs	855.12	Joback Method
dvisc	0.0000281	Paxs	925.11	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=U292351&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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