

4-Ethylbenzoic acid, heptyl ester

Inchi:	InChI=1S/C16H24O2/c1-3-5-6-7-8-13-18-16(17)15-11-9-14(4-2)10-12-15/h9-12H,3-8,13H
InchiKey:	KIXHMWSRVRBCBX-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	-47.30	kJ/mol	Joback Method
hf	-393.31	kJ/mol	Joback Method
hfus	33.63	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.376		Crippen Method
mvol	219.980	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1908.70		NIST Webbook
rinpol	1908.70		NIST Webbook
tb	673.43	K	Joback Method
tc	869.56	K	Joback Method
tf	381.18	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.73	J/molxK	673.43	Joback Method
cpg	616.73	J/molxK	706.12	Joback Method
cpg	632.81	J/molxK	738.81	Joback Method
cpg	647.97	J/molxK	771.49	Joback Method
cpg	662.26	J/molxK	804.18	Joback Method
cpg	675.69	J/molxK	836.87	Joback Method
cpg	688.29	J/molxK	869.56	Joback Method
dvisc	0.0014273	Paxs	381.18	Joback Method

dvisc	0.0007494	Paxs	429.89	Joback Method
dvisc	0.0004486	Paxs	478.60	Joback Method
dvisc	0.0002953	Paxs	527.31	Joback Method
dvisc	0.0002086	Paxs	576.01	Joback Method
dvisc	0.0001555	Paxs	624.72	Joback Method
dvisc	0.0001210	Paxs	673.43	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=U292343&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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