

4-Ethylbenzoic acid, undec-2-enyl ester

Inchi:	InChI=1S/C20H30O2/c1-3-5-6-7-8-9-10-11-12-17-22-20(21)19-15-13-18(4-2)14-16-19/h
InchiKey:	NZVPQTGCKTYURJ-VAWYXSNFSA-N
Formula:	C20H30O2
SMILES:	CCCCCCCC=CCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	302.45

Physical Properties

Property code	Value	Unit	Source
gf	66.60	kJ/mol	Joback Method
hf	-358.65	kJ/mol	Joback Method
hfus	44.20	kJ/mol	Joback Method
hvap	72.17	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.713		Crippen Method
mvol	272.040	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	2324.30		NIST Webbook
rinpol	2324.30		NIST Webbook
tb	769.11	K	Joback Method
tc	965.51	K	Joback Method
tf	421.18	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.66	J/molxK	769.11	Joback Method
cpg	819.38	J/molxK	801.84	Joback Method
cpg	836.08	J/molxK	834.58	Joback Method
cpg	851.81	J/molxK	867.31	Joback Method
cpg	866.61	J/molxK	900.04	Joback Method
cpg	880.53	J/molxK	932.78	Joback Method
cpg	893.60	J/molxK	965.51	Joback Method
dvisc	0.0009691	Paxs	421.18	Joback Method

dvisc	0.0004698	Paxs	479.17	Joback Method
dvisc	0.0002662	Paxs	537.16	Joback Method
dvisc	0.0001686	Paxs	595.14	Joback Method
dvisc	0.0001157	Paxs	653.13	Joback Method
dvisc	0.0000845	Paxs	711.12	Joback Method
dvisc	0.0000647	Paxs	769.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292548&Units=SI
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

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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