

4-Ethylbenzoic acid, tridecyl ester

Inchi:	InChI=1S/C22H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-19-24-22(23)21-17-15-20(4-2)16-18
InchiKey:	AQNSHAJHSGGDKW-UHFFFAOYSA-N
Formula:	C22H36O2
SMILES:	CCCCCCCCCCCCOC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	332.52

Physical Properties

Property code	Value	Unit	Source
gf	3.22	kJ/mol	Joback Method
hf	-517.15	kJ/mol	Joback Method
hfus	49.17	kJ/mol	Joback Method
hvap	76.66	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.717		Crippen Method
mvol	304.520	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2502.20		NIST Webbook
rinpol	2502.20		NIST Webbook
tb	810.71	K	Joback Method
tc	1003.02	K	Joback Method
tf	448.80	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.18	J/molxK	810.71	Joback Method
cpg	1027.96	J/molxK	970.97	Joback Method
cpg	1013.45	J/molxK	938.92	Joback Method
cpg	997.95	J/molxK	906.87	Joback Method
cpg	981.43	J/molxK	874.81	Joback Method
cpg	963.86	J/molxK	842.76	Joback Method
cpg	1041.52	J/molxK	1003.02	Joback Method
dvisc	0.0000571	Paxs	810.71	Joback Method

dvisc	0.0000749	Paxs	750.39	Joback Method
dvisc	0.0001030	Paxs	690.07	Joback Method
dvisc	0.0001505	Paxs	629.75	Joback Method
dvisc	0.0002383	Paxs	569.44	Joback Method
dvisc	0.0004208	Paxs	509.12	Joback Method
dvisc	0.0008656	Paxs	448.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292347&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
mccvol:	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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