Fumaric acid, 3-ethylphenyl propyl ester

Inchi: InChI=1S/C15H18O4/c1-3-10-18-14(16)8-9-15(17)19-13-7-5-6-12(4-2)11-13/h5-9,11H,3-
InchiKey: MALJFZVGSXZHRF-CMDGGOBGSA-N
Formula: C15H18O4
SMILES: CCCOC(=O)C=CC(=O)Oc1cccc(CC)c1
Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-209.42	kJ/mol	Joback Method
hf	-500.25	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	70.19	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.664		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1977.00		NIST Webbook
tb	731.00	K	Joback Method
tc	941.42	K	Joback Method
tf	436.99	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.67	J/mol×K	731.00	Joback Method
cpg	583.91	J/mol×K	766.07	Joback Method
cpg	597.21	J/mol×K	801.14	Joback Method
cpg	609.60	J/mol×K	836.21	Joback Method
cpg	621.10	J/mol×K	871.28	Joback Method
cpg	631.74	J/mol×K	906.35	Joback Method
cpg	641.54	J/mol×K	941.42	Joback Method
dvisc	0.0008463	Pa×s	436.99	Joback Method
dvisc	0.0004844	Pa×s	485.99	Joback Method

dvisc	0.0003071	Pa×s	534.99	Joback Method
dvisc	0.0002102	Pa×s	584.00	Joback Method
dvisc	0.0001526	Pa×s	633.00	Joback Method
dvisc	0.0001160	Pa×s	682.00	Joback Method
dvisc	0.0000914	Pa×s	731.00	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=U348158&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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