Fumaric acid, 3,5-dimethylphenyl 2-ethylhexyl ester

Inchi: InChI=1S/C20H28O4/c1-5-7-8-17(6-2)14-23-19(21)9-10-20(22)24-18-12-15(3)11-16(4)13

InchiKey: WSDNHSPDPXRVKI-MDZDMXLPSA-N

Formula: C20H28O4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 332.43

Physical Properties

Property code	Value	Unit	Source
gf	-179.39	kJ/mol	Joback Method
hf	-620.20	kJ/mol	Joback Method
hfus	43.07	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.525		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2414.00		NIST Webbook
tb	849.94	K	Joback Method
tc	1056.88	K	Joback Method
tf	490.86	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.04	J/mol×K	849.94	Joback Method
cpg	866.76	J/mol×K	884.43	Joback Method
cpg	881.38	J/mol×K	918.92	Joback Method
cpg	894.91	J/mol×K	953.41	Joback Method
cpg	907.40	J/mol×K	987.90	Joback Method
cpg	918.87	J/mol×K	1022.39	Joback Method
cpg	929.34	J/mol×K	1056.88	Joback Method
dvisc	0.0005271	Pa×s	490.86	Joback Method
dvisc	0.0002789	Pa×s	550.71	Joback Method

dvisc	0.0001672	Pa×s	610.55	Joback Method
dvisc	0.0001098	Pa×s	670.40	Joback Method
dvisc	0.0000773	Pa×s	730.25	Joback Method
dvisc	0.0000573	Pa×s	790.09	Joback Method
dvisc	0.0000444	Pa×s	849.94	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=U405740&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