Fumaric acid, 2-isopropylphenyl 2-ethylhexyl ester

Inchi: InChI=1S/C21H30O4/c1-5-7-10-17(6-2)15-24-20(22)13-14-21(23)25-19-12-9-8-11-18(19

InchiKey: YJZHPTOLPYRRIO-BUHFOSPRSA-N

Formula: C21H30O4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-163.78	kJ/mol	Joback Method
hf	-634.65	kJ/mol	Joback Method
hfus	42.53	kJ/mol	Joback Method
hvap	82.77	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.031		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	867.40	K	Joback Method
tc	1075.64	K	Joback Method
tf	474.61	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.29	J/mol×K	867.40	Joback Method
cpg	927.41	J/mol×K	902.11	Joback Method
cpg	942.36	J/mol×K	936.81	Joback Method
cpg	956.18	J/mol×K	971.52	Joback Method
cpg	968.91	J/mol×K	1006.23	Joback Method
cpg	980.59	J/mol×K	1040.93	Joback Method
cpg	991.25	J/mol×K	1075.64	Joback Method
dvisc	0.0006444	Pa×s	474.61	Joback Method

dvisc	0.0002951	Pa×s	540.08	Joback Method
dvisc	0.0001600	Pa×s	605.54	Joback Method
dvisc	0.0000977	Pa×s	671.00	Joback Method
dvisc	0.0000652	Pa×s	736.47	Joback Method
dvisc	0.0000464	Pa×s	801.93	Joback Method
dvisc	0.0000348	Pa×s	867.40	Joback Method

Sources

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=U405869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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