

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.29	J/molxK	867.40	Joback Method
cpg	980.59	J/molxK	1040.93	Joback Method
cpg	968.91	J/molxK	1006.23	Joback Method
cpg	956.18	J/molxK	971.52	Joback Method
cpg	942.36	J/molxK	936.81	Joback Method
cpg	927.41	J/molxK	902.11	Joback Method
cpg	991.25	J/molxK	1075.64	Joback Method
dvisc	0.0000348	Paxs	867.40	Joback Method

dvisc	0.0000464	Paxs	801.93	Joback Method
dvisc	0.0000652	Paxs	736.47	Joback Method
dvisc	0.0000977	Paxs	671.00	Joback Method
dvisc	0.0001600	Paxs	605.54	Joback Method
dvisc	0.0002951	Paxs	540.08	Joback Method
dvisc	0.0006444	Paxs	474.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405869&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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