

Fumaric acid, 3-phenylpropyl 2-ethylhexyl ester

Inchi:	InChI=1S/C21H30O4/c1-3-5-10-18(4-2)17-25-21(23)15-14-20(22)24-16-9-13-19-11-7-6-8
InchiKey:	ICMHFGNKYPKMBQ-CCEZHUSRSA-N
Formula:	C21H30O4
SMILES:	CCCCC(CC)COC(=O)C=CC(=O)OCCCC1CCCCC1
Mol. weight [g/mol]:	346.46

Physical Properties

Property code	Value	Unit	Source
gf	-151.71	kJ/mol	Joback Method
hf	-617.90	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	82.50	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.478		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2527.00		NIST Webbook
tb	862.86	K	Joback Method
tc	1068.44	K	Joback Method
tf	477.09	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.48	J/molxK	862.86	Joback Method
cpg	927.57	J/molxK	897.12	Joback Method
cpg	942.51	J/molxK	931.39	Joback Method
cpg	956.37	J/molxK	965.65	Joback Method
cpg	969.18	J/molxK	999.91	Joback Method
cpg	980.98	J/molxK	1034.17	Joback Method
cpg	991.83	J/molxK	1068.44	Joback Method
dvisc	0.0006671	Paxs	477.09	Joback Method
dvisc	0.0003105	Paxs	541.38	Joback Method

dvisc	0.0001700	Paxs	605.68	Joback Method
dvisc	0.0001045	Paxs	669.97	Joback Method
dvisc	0.0000700	Paxs	734.27	Joback Method
dvisc	0.0000499	Paxs	798.56	Joback Method
dvisc	0.0000375	Paxs	862.86	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=U405667&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

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