Fumaric acid, isohexyl 2-propylphenyl ester

Inchi: InChI=1S/C19H26O4/c1-4-8-16-10-5-6-11-17(16)23-19(21)13-12-18(20)22-14-7-9-15(2)3
InchiKey: XIZVTGZKYMHQEY-OUKQBFOZSA-N
Formula: C19H26O4
SMILES: CCCc1ccccc1OC(=O)C=CC(=O)OCCCC(C)C
Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-178.18	kJ/mol	Joback Method
hf	-588.09	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	78.71	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.080		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook
tb	822.08	K	Joback Method
tc	1028.56	K	Joback Method
tf	467.07	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.60	J/mol×K	822.08	Joback Method
cpg	809.20	J/mol×K	856.49	Joback Method
cpg	823.72	J/mol×K	890.91	Joback Method
cpg	837.19	J/mol×K	925.32	Joback Method
cpg	849.65	J/mol×K	959.74	Joback Method
cpg	861.13	J/mol×K	994.15	Joback Method
cpg	871.66	J/mol×K	1028.56	Joback Method
dvisc	0.0006893	Pa×s	467.07	Joback Method

dvisc	0.0003486	Pa×s	526.24	Joback Method
dvisc	0.0002023	Pa×s	585.41	Joback Method
dvisc	0.0001298	Pa×s	644.57	Joback Method
dvisc	0.0000897	Pa×s	703.74	Joback Method
dvisc	0.0000656	Pa×s	762.91	Joback Method
dvisc	0.0000503	Pa×s	822.08	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=U348128&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