Fumaric acid, 3-phenylpropyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C18H24O4/c1-14(2)15(3)22-18(20)12-11-17(19)21-13-7-10-16-8-5-4-6-9-16/h4

InchiKey: ZHMLFTLVMAJOHS-VAWYXSNFSA-N

Formula: C18H24O4

SMILES: CC(C)C(C)OC(=O)C=CC(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	-179.41	kJ/mol	Joback Method
hf	-561.26	kJ/mol	Joback Method
hfus	35.15	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.306		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	793.78	K	Joback Method
tc	1003.25	K	Joback Method
tf	428.28	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.65	J/mol×K	793.78	Joback Method
cpg	753.32	J/mol×K	828.69	Joback Method
cpg	767.89	J/mol×K	863.60	Joback Method
cpg	781.40	J/mol×K	898.52	Joback Method
cpg	793.88	J/mol×K	933.43	Joback Method
cpg	805.37	J/mol×K	968.34	Joback Method
cpg	815.92	J/mol×K	1003.25	Joback Method
dvisc	0.0010956	Pa×s	428.28	Joback Method

dvisc	0.0004816	Pa×s	489.20	Joback Method
dvisc	0.0002539	Pa×s	550.11	Joback Method
dvisc	0.0001521	Pa×s	611.03	Joback Method
dvisc	0.0001000	Pa×s	671.95	Joback Method
dvisc	0.0000705	Pa×s	732.86	Joback Method
dvisc	0.0000524	Pa×s	793.78	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=U405661&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