Fumaric acid, 3,4-dimethylphenyl hexyl ester

Inchi: InChI=1S/C18H24O6/c1-4-5-6-7-12-23-17(19)10-11-18(20)24-14-8-9-15(21-2)16(13-14)2
InchiKey: IQCCMXKQRJZZHR-ZHACJKMWSA-N
Formula: C18H24O6
SMILES: CCCCCCOC(=O)C=CC(=O)Oc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-403.79	kJ/mol	Joback Method
hf	-838.08	kJ/mol	Joback Method
hfus	43.79	kJ/mol	Joback Method
hvap	82.35	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.289		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
tb	849.46	K	Joback Method
tc	1055.39	K	Joback Method
tf	527.78	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.06	J/mol×K	849.46	Joback Method
cpg	850.58	J/mol×K	1021.06	Joback Method
cpg	840.97	J/mol×K	986.74	Joback Method
cpg	830.21	J/mol×K	952.42	Joback Method
cpg	818.30	J/mol×K	918.10	Joback Method
cpg	805.25	J/mol×K	883.78	Joback Method
cpg	859.03	J/mol×K	1055.39	Joback Method
dvisc	0.0000362	Pa×s	849.46	Joback Method

dvisc	0.0000455	Pa×s	795.85	Joback Method
dvisc	0.0000591	Pa×s	742.23	Joback Method
dvisc	0.0000801	Pa×s	688.62	Joback Method
dvisc	0.0001142	Pa×s	635.01	Joback Method
dvisc	0.0001738	Pa×s	581.39	Joback Method
dvisc	0.0002882	Pa×s	527.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348169&Units=SI

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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