Fumaric acid, 3,5-dimethylphenyl hept-2-yl ester

Inchi: InChI=1S/C19H26O4/c1-5-6-7-8-16(4)22-18(20)9-10-19(21)23-17-12-14(2)11-15(3)13-17

InchiKey: JCARGHJGCCDSPX-MDZDMXLPSA-N

Formula: C19H26O4

SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 318.41

Physical Properties

Property code	Value	Unit	Source
gf	-187.81	kJ/mol	Joback Method
hf	-599.56	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.277		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2296.00		NIST Webbook
tb	827.06	K	Joback Method
tc	1034.35	K	Joback Method
tf	479.59	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.80	J/mol×K	827.06	Joback Method
cpg	859.88	J/mol×K	999.80	Joback Method
cpg	848.51	J/mol×K	965.25	Joback Method
cpg	836.14	J/mol×K	930.71	Joback Method
cpg	822.75	J/mol×K	896.16	Joback Method
cpg	808.32	J/mol×K	861.61	Joback Method
cpg	870.29	J/mol×K	1034.35	Joback Method
dvisc	0.0000508	Pa×s	827.06	Joback Method
dvisc	0.0000655	Pa×s	769.15	Joback Method

dvisc	0.0000879	Pa×s	711.24	Joback Method
dvisc	0.0001243	Pa×s	653.33	Joback Method
dvisc	0.0001880	Pa×s	595.41	Joback Method
dvisc	0.0003110	Pa×s	537.50	Joback Method
dvisc	0.0005809	Pa×s	479.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405739&Units=SI
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

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