

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-MDZDMLPSA-N
Formula:	C19H26O4
SMILES:	CCCCC(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
rinqol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.80	J/molxK	827.06	Joback Method
cpg	808.32	J/molxK	861.61	Joback Method
cpg	822.75	J/molxK	896.16	Joback Method
cpg	836.14	J/molxK	930.71	Joback Method
cpg	848.51	J/molxK	965.25	Joback Method
cpg	859.88	J/molxK	999.80	Joback Method
cpg	870.29	J/molxK	1034.35	Joback Method
dvisc	0.0005809	Paxs	479.59	Joback Method
dvisc	0.0003110	Paxs	537.50	Joback Method

dvisc	0.0001880	Paxs	595.41	Joback Method
dvisc	0.0001243	Paxs	653.33	Joback Method
dvisc	0.0000879	Paxs	711.24	Joback Method
dvisc	0.0000655	Paxs	769.15	Joback Method
dvisc	0.0000508	Paxs	827.06	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/ci9903071
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

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