Fumaric acid, 3,5-dimethylphenyl cyclohexylmethyl ester

Inchi: InChI=1S/C19H24O4/c1-14-10-15(2)12-17(11-14)23-19(21)9-8-18(20)22-13-16-6-4-3-5-7

InchiKey: CNHYTYRDSMWFHU-CMDGGOBGSA-N

Formula: C19H24O4

SMILES: Cc1cc(C)cc(OC(=O)C=CC(=O)OCC2CCCCC2)c1

Mol. weight [g/mol]: 316.39

Physical Properties

Property code	Value	Unit	Source
gf	-160.92	kJ/mol	Joback Method
hf	-539.96	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.889		Crippen Method
mcvol	254.530	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2490.00		NIST Webbook
tb	847.05	K	Joback Method
tc	1075.20	K	Joback Method
tf	501.97	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.70	J/mol×K	847.05	Joback Method
cpg	855.23	J/mol×K	1037.18	Joback Method
cpg	844.22	J/mol×K	999.15	Joback Method
cpg	831.90	J/mol×K	961.13	Joback Method
cpg	818.24	J/mol×K	923.10	Joback Method
cpg	803.18	J/mol×K	885.08	Joback Method
cpg	864.97	J/mol×K	1075.20	Joback Method
dvisc	0.0000576	Pa×s	847.05	Joback Method
dvisc	0.0000737	Pa×s	789.54	Joback Method

dvisc	0.0000981	Pa×s	732.02	Joback Method
dvisc	0.0001370	Pa×s	674.51	Joback Method
dvisc	0.0002036	Pa×s	617.00	Joback Method
dvisc	0.0003282	Pa×s	559.48	Joback Method
dvisc	0.0005905	Pa×s	501.97	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=U405741&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