Fumaric acid, 3,5-dimethylphenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H20O4/c1-12(2)7-8-20-16(18)5-6-17(19)21-15-10-13(3)9-14(4)11-15/h5-7,

InchiKey: KQAJNWXUHZXHHY-AATRIKPKSA-N

Formula: C17H20O4

SMILES: CC(C)=CCOC(=O)C=CC(=O)Oc1cc(C)cc(C)c1

Mol. weight [g/mol]: 288.34

Physical Properties

Property code	Value	Unit	Source
gf	-130.54	kJ/mol	Joback Method
hf	-445.57	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	75.34	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.274		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	785.78	K	Joback Method
tc	1001.61	K	Joback Method
tf	453.01	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.71	J/mol×K	785.78	Joback Method
cpg	667.18	J/mol×K	821.75	Joback Method
cpg	680.69	J/mol×K	857.72	Joback Method
cpg	693.27	J/mol×K	893.70	Joback Method
cpg	704.96	J/mol×K	929.67	Joback Method
cpg	715.79	J/mol×K	965.64	Joback Method
cpg	725.80	J/mol×K	1001.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405737&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
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