

Fumaric acid, 3-phenylpropyl 3-methylbut-2-en-1-yl ester

Inchi:	InChI=1S/C18H22O4/c1-15(2)12-14-22-18(20)11-10-17(19)21-13-6-9-16-7-4-3-5-8-16/h3
InchiKey:	UTNFDMGXEPZAMD-ZHACJKMWSA-N
Formula:	C18H22O4
SMILES:	CC(C)=CCOC(=O)C=CC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	302.36

Physical Properties

Property code	Value	Unit	Source
gf	-102.86	kJ/mol	Joback Method
hf	-443.27	kJ/mol	Joback Method
hfus	41.09	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.228		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	798.70	K	Joback Method
tc	1010.88	K	Joback Method
tf	439.24	K	Joback Method
vc	0.945	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.60	J/mol×K	798.70	Joback Method
cpg	725.54	J/mol×K	834.06	Joback Method
cpg	739.48	J/mol×K	869.43	Joback Method
cpg	752.45	J/mol×K	904.79	Joback Method
cpg	764.52	J/mol×K	940.15	Joback Method
cpg	775.74	J/mol×K	975.51	Joback Method
cpg	786.17	J/mol×K	1010.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U405663&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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