

o-anisic acid, 3-methylbut-2-enyl ester

Inchi:	InChI=1S/C13H16O3/c1-10(2)8-9-16-13(14)11-6-4-5-7-12(11)15-3/h4-8H,9H2,1-3H3
InchiKey:	NVWMLQUAAXVRQY-UHFFFAOYSA-N
Formula:	C13H16O3
SMILES:	COc1ccccc1C(=O)OCC=C(C)C
Mol. weight [g/mol]:	220.27

Physical Properties

Property code	Value	Unit	Source
hf	-416.94	kJ/mol	Cheméo Relay (1.0)
hfus	25.95	kJ/mol	Joback Method
hvap	75.90	kJ/mol	Cheméo Relay (1.0)
ie	8.18	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	2.818		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1722.20		NIST Webbook
rinpol	1722.20		NIST Webbook
tb	571.59	K	Cheméo Relay (1.0)
tf	282.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.06	J/mol×K	631.25	Joback Method
cpg	463.02	J/mol×K	666.83	Joback Method
cpg	477.11	J/mol×K	702.41	Joback Method
cpg	490.35	J/mol×K	738.00	Joback Method
cpg	502.76	J/mol×K	773.58	Joback Method
cpg	514.36	J/mol×K	809.16	Joback Method
cpg	525.17	J/mol×K	844.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292572&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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