

Fumaric acid, di(4-methylpent-2-yl) ester

Inchi:	InChI=1S/C16H28O4/c1-11(2)9-13(5)19-15(17)7-8-16(18)20-14(6)10-12(3)4/h7-8,11-14H
InchiKey:	NZQQFMVULBBDSP-BQYQJAHWSA-N
Formula:	C16H28O4
SMILES:	CC(C)CC(C)OC(=O)C=CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-313.54	kJ/mol	Joback Method
hf	-767.07	kJ/mol	Joback Method
hfus	28.88	kJ/mol	Joback Method
hvap	67.93	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.498		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	720.46	K	Joback Method
tc	910.25	K	Joback Method
tf	349.32	K	Joback Method
vc	0.935	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.39	J/molxK	720.46	Joback Method
cpg	729.33	J/molxK	752.09	Joback Method
cpg	745.35	J/molxK	783.72	Joback Method
cpg	760.46	J/molxK	815.36	Joback Method
cpg	774.67	J/molxK	846.99	Joback Method
cpg	788.01	J/molxK	878.62	Joback Method
cpg	800.49	J/molxK	910.25	Joback Method
dvisc	0.0030382	Paxs	349.32	Joback Method

dvisc	0.0009576	Paxs	411.18	Joback Method
dvisc	0.0004082	Paxs	473.03	Joback Method
dvisc	0.0002119	Paxs	534.89	Joback Method
dvisc	0.0001261	Paxs	596.75	Joback Method
dvisc	0.0000827	Paxs	658.60	Joback Method
dvisc	0.0000583	Paxs	720.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348332&Units=SI
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

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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