Fumaric acid, di(2-methylpent-3-yl) ester

Inchi: InChI=1S/C16H28O4/c1-7-13(11(3)4)19-15(17)9-10-16(18)20-14(8-2)12(5)6/h9-14H,7-8H
InchiKey: WQXYJBHHPWLNAO-MDZDMXLPSA-N
Formula: C16H28O4
SMILES: CCC(OC(=O)C=CC(=O)OC(CC)C(C)C)C(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	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	720.46	K	Joback Method
tc	910.25	K	Joback Method
tf	349.32	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.39	J/mol×K	720.46	Joback Method
cpg	788.01	J/mol×K	878.62	Joback Method
cpg	774.67	J/mol×K	846.99	Joback Method
cpg	760.46	J/mol×K	815.36	Joback Method
cpg	745.35	J/mol×K	783.72	Joback Method
cpg	729.33	J/mol×K	752.09	Joback Method
cpg	800.49	J/mol×K	910.25	Joback Method
dvisc	0.0000583	Pa×s	720.46	Joback Method

dvisc	0.0000827	Pa×s	658.60	Joback Method
dvisc	0.0001261	Pa×s	596.75	Joback Method
dvisc	0.0002119	Pa×s	534.89	Joback Method
dvisc	0.0004082	Pa×s	473.03	Joback Method
dvisc	0.0009576	Pa×s	411.18	Joback Method
dvisc	0.0030382	Pa×s	349.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348777&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
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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