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

Inchi: InChI=1S/C16H28O4/c1-11(15(3,4)5)19-13(17)9-10-14(18)20-12(2)16(6,7)8/h9-12H,1-8H
InchiKey: KWLHKXVMTJVPQF-MDZDMXLPSA-N
Formula: C16H28O4
SMILES: CC(OC(=O)C=CC(=O)OC(C)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-302.98	kJ/mol	Joback Method
hf	-774.01	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.498		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	714.88	K	Joback Method
tc	914.84	K	Joback Method
tf	384.16	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.75	J/mol×K	714.88	Joback Method
cpg	792.19	J/mol×K	881.51	Joback Method
cpg	778.81	J/mol×K	848.19	Joback Method
cpg	764.53	J/mol×K	814.86	Joback Method
cpg	749.30	J/mol×K	781.53	Joback Method
cpg	733.05	J/mol×K	748.21	Joback Method
cpg	804.72	J/mol×K	914.84	Joback Method
dvisc	0.0000475	Pa×s	714.88	Joback Method

dvisc	0.0000682	Pa×s	659.76	Joback Method
dvisc	0.0001044	Pa×s	604.64	Joback Method
dvisc	0.0001743	Pa×s	549.52	Joback Method
dvisc	0.0003260	Pa×s	494.40	Joback Method
dvisc	0.0007135	Pa×s	439.28	Joback Method
dvisc	0.0019554	Pa×s	384.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348720&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