Fumaric acid, 3,3-dimethylbut-2-yl nonyl ester

Inchi: InChI=1S/C19H34O4/c1-6-7-8-9-10-11-12-15-22-17(20)13-14-18(21)23-16(2)19(3,4)5/h1
InchiKey: IWSPJLGLQVEGTK-BUHFOSPRSA-N
Formula: C19H34O4
SMILES: CCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-278.12	kJ/mol	Joback Method
hf	-821.90	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	74.47	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.814		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	787.19	K	Joback Method
tc	976.25	K	Joback Method
tf	430.55	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.91	J/mol×K	787.19	Joback Method
cpg	963.91	J/mol×K	944.74	Joback Method
cpg	950.15	J/mol×K	913.23	Joback Method
cpg	935.51	J/mol×K	881.72	Joback Method
cpg	919.95	J/mol×K	850.21	Joback Method
cpg	903.43	J/mol×K	818.70	Joback Method
cpg	976.82	J/mol×K	976.25	Joback Method
dvisc	0.0000396	Pa×s	787.19	Joback Method

dvisc	0.0000546	Pa×s	727.75	Joback Method
dvisc	0.0000796	Pa×s	668.31	Joback Method
dvisc	0.0001251	Pa×s	608.87	Joback Method
dvisc	0.0002166	Pa×s	549.43	Joback Method
dvisc	0.0004286	Pa×s	489.99	Joback Method
dvisc	0.0010237	Pa×s	430.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348708&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