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

Inchi: InChI=1S/C20H36O4/c1-6-7-8-9-10-11-12-13-16-23-18(21)14-15-19(22)24-17(2)20(3,4)5

InchiKey: CETPITKVFMBCFW-CCEZHUSRSA-N

Formula: C20H36O4

SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-269.70	kJ/mol	Joback Method
hf	-842.54	kJ/mol	Joback Method
hfus	42.39	kJ/mol	Joback Method
hvap	76.70	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.204		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	810.07	K	Joback Method
tc	1000.27	K	Joback Method
tf	441.82	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.41	J/mol×K	810.07	Joback Method
cpg	1024.63	J/mol×K	968.57	Joback Method
cpg	1010.68	J/mol×K	936.87	Joback Method
cpg	995.83	J/mol×K	905.17	Joback Method
cpg	980.02	J/mol×K	873.47	Joback Method
cpg	963.23	J/mol×K	841.77	Joback Method
cpg	1037.72	J/mol×K	1000.27	Joback Method
dvisc	0.0000340	Pa×s	810.07	Joback Method

dvisc	0.0000470	Pa×s	748.69	Joback Method
dvisc	0.0000687	Pa×s	687.32	Joback Method
dvisc	0.0001082	Pa×s	625.94	Joback Method
dvisc	0.0001881	Pa×s	564.57	Joback Method
dvisc	0.0003743	Pa×s	503.20	Joback Method
dvisc	0.0009017	Pa×s	441.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348709&Units=SI

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