Fumaric acid, dodecyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C20H34O5/c1-4-5-6-7-8-9-10-11-12-13-16-24-19(22)14-15-20(23)25-18(3)17(2
InchiKey: TYYXXOUHSFLVKB-CCEZHUSRSA-N
Formula: C20H34O5
SMILES: CCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 354.48

Physical Properties

Property code	Value	Unit	Source
gf	-401.46	kJ/mol	Joback Method
hf	-946.37	kJ/mol	Joback Method
hfus	51.41	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.527		Crippen Method
mcvol	304.810	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook
tb	867.17	K	Joback Method
tc	1064.01	K	Joback Method
tf	489.33	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.67	J/mol×K	867.17	Joback Method
cpg	1036.70	J/mol×K	1031.21	Joback Method
cpg	1024.54	J/mol×K	998.40	Joback Method
cpg	1011.39	J/mol×K	965.59	Joback Method
cpg	997.21	J/mol×K	932.78	Joback Method
cpg	981.98	J/mol×K	899.98	Joback Method
cpg	1047.89	J/mol×K	1064.01	Joback Method
dvisc	0.0000404	Pa×s	867.17	Joback Method

dvisc	0.0000539	Pa×s	804.20	Joback Method
dvisc	0.0000755	Pa×s	741.22	Joback Method
dvisc	0.0001125	Pa×s	678.25	Joback Method
dvisc	0.0001821	Pa×s	615.28	Joback Method
dvisc	0.0003289	Pa×s	552.30	Joback Method
dvisc	0.0006917	Pa×s	489.33	Joback Method

Sources

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=U348826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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