Fumaric acid, decyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C21H38O4/c1-6-7-8-9-10-11-12-13-16-24-19(22)14-15-20(23)25-21(17(2)3)18
InchiKey: VSCNDMTYLCLTFJ-CCEZHUSRSA-N
Formula: C21H38O4
SMILES: CCCCCCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-269.00	kJ/mol	Joback Method
hf	-864.99	kJ/mol	Joback Method
hfus	45.35	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.450		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2324.00		NIST Webbook
tb	835.30	K	Joback Method
tc	1026.77	K	Joback Method
tf	420.67	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.90	J/mol×K	835.30	Joback Method
cpg	1086.64	J/mol×K	994.86	Joback Method
cpg	1072.59	J/mol×K	962.95	Joback Method
cpg	1057.52	J/mol×K	931.03	Joback Method
cpg	1041.40	J/mol×K	899.12	Joback Method
cpg	1024.21	J/mol×K	867.21	Joback Method
cpg	1099.70	J/mol×K	1026.77	Joback Method
dvisc	0.0000309	Pa×s	835.30	Joback Method
dvisc	0.0000433	Pa×s	766.19	Joback Method

dvisc	0.0000648	Pa×s	697.09	Joback Method
dvisc	0.0001059	Pa×s	627.99	Joback Method
dvisc	0.0001954	Pa×s	558.88	Joback Method
dvisc	0.0004290	Pa×s	489.77	Joback Method
dvisc	0.0012192	Pa×s	420.67	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=U348551&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