Fumaric acid, dodecyl pent-4-en-2-yl ester

Inchi: InChI=1S/C21H36O4/c1-4-6-7-8-9-10-11-12-13-14-18-24-20(22)16-17-21(23)25-19(3)15
InchiKey: UKAKBTIQXZHAAA-WUKNDPDISA-N
Formula: C21H36O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-176.28	kJ/mol	Joback Method
hf	-729.00	kJ/mol	Joback Method
hfus	51.12	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.514		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2397.00		NIST Webbook
rinpol	2397.00		NIST Webbook
tb	832.86	K	Joback Method
tc	1022.98	K	Joback Method
tf	448.91	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.48	J/mol×K	832.86	Joback Method
cpg	995.11	J/mol×K	864.55	Joback Method
cpg	1011.70	J/mol×K	896.23	Joback Method
cpg	1027.29	J/mol×K	927.92	Joback Method
cpg	1041.92	J/mol×K	959.60	Joback Method
cpg	1055.62	J/mol×K	991.29	Joback Method
cpg	1068.41	J/mol×K	1022.98	Joback Method
dvisc	0.0008337	Pa×s	448.91	Joback Method

dvisc	0.0003649	Pa×s	512.90	Joback Method
dvisc	0.0001918	Pa×s	576.89	Joback Method
dvisc	0.0001147	Pa×s	640.88	Joback Method
dvisc	0.0000752	Pa×s	704.88	Joback Method
dvisc	0.0000530	Pa×s	768.87	Joback Method
dvisc	0.0000394	Pa×s	832.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348931&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