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

Inchi: InChI=1S/C25H44O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-29-24(27)19-20-25
InchiKey: VQJZWNXAZIXVHO-FMQUCBEESA-N
Formula: C25H44O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 424.61

Physical Properties

Property code	Value	Unit	Source
gf	-359.36	kJ/mol	Joback Method
hf	-1049.57	kJ/mol	Joback Method
hfus	64.36	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.478		Crippen Method
mcvol	375.260	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	2951.00		NIST Webbook
tb	981.57	K	Joback Method
tc	1205.71	K	Joback Method
tf	545.68	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.83	J/mol×K	981.57	Joback Method
cpg	1292.26	J/mol×K	1018.93	Joback Method
cpg	1309.17	J/mol×K	1056.28	Joback Method
cpg	1324.63	J/mol×K	1093.64	Joback Method
cpg	1338.68	J/mol×K	1131.00	Joback Method
cpg	1351.40	J/mol×K	1168.35	Joback Method
cpg	1362.85	J/mol×K	1205.71	Joback Method
dvisc	0.0003703	Pa×s	545.68	Joback Method
dvisc	0.0001683	Pa×s	618.33	Joback Method

dvisc	0.0000903	Pa×s	690.98	Joback Method
dvisc	0.0000546	Pa×s	763.62	Joback Method
dvisc	0.0000360	Pa×s	836.27	Joback Method
dvisc	0.0000254	Pa×s	908.92	Joback Method
dvisc	0.0000188	Pa×s	981.57	Joback Method

Sources

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=U348831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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