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

Inchi: InChI=1S/C31H58O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-34-29(

InchiKey: BFPSTMGFNSVCDS-OCOZRVBESA-N

Formula: C31H58O4

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

Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-184.80	kJ/mol	Joback Method
hf	-1071.39	kJ/mol	Joback Method
hfus	71.25	kJ/mol	Joback Method
hvap	101.71	kJ/mol	Joback Method
log10ws	-10.01		Crippen Method
logp	9.351		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	616.95	kPa	Joback Method
rinpol	3334.00		NIST Webbook
rinpol	3334.00		NIST Webbook
tb	1064.10	K	Joback Method
tc	1331.02	K	Joback Method
tf	533.37	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.99	J/mol×K	1064.10	Joback Method
cpg	1739.32	J/mol×K	1286.53	Joback Method
cpg	1724.06	J/mol×K	1242.05	Joback Method
cpg	1706.94	J/mol×K	1197.56	Joback Method
cpg	1687.81	J/mol×K	1153.07	Joback Method
cpg	1666.55	J/mol×K	1108.59	Joback Method
cpg	1752.88	J/mol×K	1331.02	Joback Method
dvisc	0.0000064	Pa×s	1064.10	Joback Method

dvisc	0.0000091	Pa×s	975.64	Joback Method
dvisc	0.0000137	Pa×s	887.19	Joback Method
dvisc	0.0000227	Pa×s	798.73	Joback Method
dvisc	0.0000428	Pa×s	710.28	Joback Method
dvisc	0.0000964	Pa×s	621.83	Joback Method
dvisc	0.0002844	Pa×s	533.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348561&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

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