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

Inchi: InChI=1S/C24H44O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-27-22(25)17-18-23(26)28-24(

InchiKey: BLSQXBNOSWJHOM-ISLYRVAYSA-N

Formula: C24H44O4

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

Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-243.74	kJ/mol	Joback Method
hf	-926.91	kJ/mol	Joback Method
hfus	53.12	kJ/mol	Joback Method
hvap	86.12	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	6.621		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		NIST Webbook
tb	903.94	K	Joback Method
tc	1106.68	K	Joback Method
tf	454.48	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.81	J/mol×K	903.94	Joback Method
cpg	1276.18	J/mol×K	1072.89	Joback Method
cpg	1261.75	J/mol×K	1039.10	Joback Method
cpg	1246.14	J/mol×K	1005.31	Joback Method
cpg	1229.31	J/mol×K	971.52	Joback Method
cpg	1211.22	J/mol×K	937.73	Joback Method
cpg	1289.48	J/mol×K	1106.68	Joback Method
dvisc	0.0000196	Pa×s	903.94	Joback Method

dvisc	0.0000275	Pa×s	829.03	Joback Method
dvisc	0.0000414	Pa×s	754.12	Joback Method
dvisc	0.0000680	Pa×s	679.21	Joback Method
dvisc	0.0001264	Pa×s	604.30	Joback Method
dvisc	0.0002799	Pa×s	529.39	Joback Method
dvisc	0.0008059	Pa×s	454.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348554&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