Fumaric acid, hexadecyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C26H48O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-29-25(27)19-20-26(2

InchiKey: RUVKRQMNXXVTBY-FMQUCBEESA-N

Formula: C26H48O4

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

Mol. weight [g/mol]: 424.66

Physical Properties

Property code	Value	Unit	Source
gf	-224.46	kJ/mol	Joback Method
hf	-962.91	kJ/mol	Joback Method
hfus	61.83	kJ/mol	Joback Method
hvap	90.96	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	7.545		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	791.71	kPa	Joback Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook
tb	950.14	K	Joback Method
tc	1166.06	K	Joback Method
tf	492.02	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.29	J/mol×K	950.14	Joback Method
cpg	1338.75	J/mol×K	986.13	Joback Method
cpg	1357.70	J/mol×K	1022.11	Joback Method
cpg	1375.21	J/mol×K	1058.10	Joback Method
cpg	1391.34	J/mol×K	1094.09	Joback Method
cpg	1406.15	J/mol×K	1130.08	Joback Method
cpg	1419.70	J/mol×K	1166.06	Joback Method
dvisc	0.0005087	Pa×s	492.02	Joback Method

dvisc	0.0001932	Pa×s	568.37	Joback Method
dvisc	0.0000922	Pa×s	644.73	Joback Method
dvisc	0.0000515	Pa×s	721.08	Joback Method
dvisc	0.0000322	Pa×s	797.43	Joback Method
dvisc	0.0000218	Pa×s	873.79	Joback Method
dvisc	0.0000157	Pa×s	950.14	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=U348330&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