Fumaric acid, heptadecyl pent-4-enyl ester

Inchi: InChI=1S/C26H46O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20-24-30-26(28)22-21-2
InchiKey: QFSBOZNLRZNHOX-QURGRASLSA-N
Formula: C26H46O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-131.74	kJ/mol	Joback Method
hf	-826.92	kJ/mol	Joback Method
hfus	67.59	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.467		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	803.42	kPa	Joback Method
rinpol	2978.00		NIST Webbook
rinpol	2978.00		NIST Webbook
tb	947.70	K	Joback Method
tc	1163.86	K	Joback Method
tf	520.26	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.87	J/mol×K	947.70	Joback Method
cpg	1375.11	J/mol×K	1127.83	Joback Method
cpg	1360.22	J/mol×K	1091.80	Joback Method
cpg	1344.12	J/mol×K	1055.78	Joback Method
cpg	1326.74	J/mol×K	1019.75	Joback Method
cpg	1308.01	J/mol×K	983.73	Joback Method
cpg	1388.86	J/mol×K	1163.86	Joback Method
dvisc	0.0000204	Pa×s	947.70	Joback Method

dvisc	0.0000274	Pa×s	876.46	Joback Method
dvisc	0.0000386	Pa×s	805.22	Joback Method
dvisc	0.0000582	Pa×s	733.98	Joback Method
dvisc	0.0000958	Pa×s	662.74	Joback Method
dvisc	0.0001780	Pa×s	591.50	Joback Method
dvisc	0.0003916	Pa×s	520.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348857&Units=SI

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