Fumaric acid, cis-non-3-enyl propyl ester

Inchi: InChI=1S/C16H26O4/c1-3-5-6-7-8-9-10-14-20-16(18)12-11-15(17)19-13-4-2/h8-9,11-12H
InchiKey: CGTOJJPEEONSGI-UONSLQGUSA-N
Formula: C16H26O4
SMILES: CCCCCC=CCCOC(=O)C=CC(=O)OCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-223.56	kJ/mol	Joback Method
hf	-628.73	kJ/mol	Joback Method
hfus	43.17	kJ/mol	Joback Method
hvap	69.44	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	726.38	K	Joback Method
tc	911.77	K	Joback Method
tf	404.24	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.97	J/mol×K	726.38	Joback Method
cpg	702.52	J/mol×K	757.28	Joback Method
cpg	717.26	J/mol×K	788.18	Joback Method
cpg	731.22	J/mol×K	819.07	Joback Method
cpg	744.43	J/mol×K	849.97	Joback Method
cpg	756.90	J/mol×K	880.87	Joback Method
cpg	768.68	J/mol×K	911.77	Joback Method
dvisc	0.0010816	Pa×s	404.24	Joback Method

dvisc	0.0005229	Pa×s	457.93	Joback Method
dvisc	0.0002944	Pa×s	511.62	Joback Method
dvisc	0.0001849	Pa×s	565.31	Joback Method
dvisc	0.0001259	Pa×s	619.00	Joback Method
dvisc	0.0000911	Pa×s	672.69	Joback Method
dvisc	0.0000692	Pa×s	726.38	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=U348877&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