Fumaric acid, heptyl pent-4-enyl ester

Inchi: InChI=1S/C16H26O4/c1-3-5-7-8-10-14-20-16(18)12-11-15(17)19-13-9-6-4-2/h4,11-12H,2
InchiKey: SGLOUBOOSRWDAJ-VAWYXSNFSA-N
Formula: C16H26O4
SMILES: C=CCCCOC(=O)C=CC(=O)OCCCCCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-215.94	kJ/mol	Joback Method
hf	-620.52	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	68.81	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	718.90	K	Joback Method
tc	901.36	K	Joback Method
tf	407.56	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.83	J/mol×K	718.90	Joback Method
cpg	755.69	J/mol×K	870.95	Joback Method
cpg	743.24	J/mol×K	840.54	Joback Method
cpg	730.05	J/mol×K	810.13	Joback Method
cpg	716.10	J/mol×K	779.72	Joback Method
cpg	701.37	J/mol×K	749.31	Joback Method
cpg	767.42	J/mol×K	901.36	Joback Method
dvisc	0.0000846	Pa×s	718.90	Joback Method

dvisc	0.0001105	Pa×s	667.01	Joback Method
dvisc	0.0001509	Pa×s	615.12	Joback Method
dvisc	0.0002183	Pa×s	563.23	Joback Method
dvisc	0.0003403	Pa×s	511.34	Joback Method
dvisc	0.0005865	Pa×s	459.45	Joback Method
dvisc	0.0011610	Pa×s	407.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348849&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