Fumaric acid, 2-heptyl pentyl ester

Inchi: InChI=1S/C16H28O4/c1-4-6-8-10-14(3)20-16(18)12-11-15(17)19-13-9-7-5-2/h11-12,14H
InchiKey: AFJGCYSHNUYEAQ-VAWYXSNFSA-N
Formula: C16H28O4
SMILES: CCCCCOC(=O)C=CC(=O)OC(C)CCCCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-306.22	kJ/mol	Joback Method
hf	-751.23	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1901.00		NIST Webbook
tb	721.78	K	Joback Method
tc	904.51	K	Joback Method
tf	394.32	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.90	J/mol×K	721.78	Joback Method
cpg	783.99	J/mol×K	874.05	Joback Method
cpg	770.99	J/mol×K	843.60	Joback Method
cpg	757.19	J/mol×K	813.14	Joback Method
cpg	742.59	J/mol×K	782.69	Joback Method
cpg	727.17	J/mol×K	752.23	Joback Method
cpg	796.23	J/mol×K	904.51	Joback Method
dvisc	0.0000739	Pa×s	721.78	Joback Method
dvisc	0.0000989	Pa×s	667.20	Joback Method

dvisc	0.0001394	Pa×s	612.63	Joback Method
dvisc	0.0002100	Pa×s	558.05	Joback Method
dvisc	0.0003457	Pa×s	503.47	Joback Method
dvisc	0.0006427	Pa×s	448.90	Joback Method
dvisc	0.0014186	Pa×s	394.32	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=U348624&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