Fumaric acid, heptyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C16H26O4/c1-4-5-6-7-8-12-19-15(17)9-10-16(18)20-13-11-14(2)3/h9-10H,2,4-
InchiKey: QGYGNMSZHBNWCH-MDZDMXLPSA-N
Formula: C16H26O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCCC
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	-224.49	kJ/mol	Joback Method
hf	-630.31	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	718.78	K	Joback Method
tc	903.14	K	Joback Method
tf	393.60	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.50	J/mol×K	718.78	Joback Method
cpg	701.18	J/mol×K	749.51	Joback Method
cpg	716.04	J/mol×K	780.23	Joback Method
cpg	730.11	J/mol×K	810.96	Joback Method
cpg	743.41	J/mol×K	841.69	Joback Method
cpg	755.95	J/mol×K	872.41	Joback Method
cpg	767.77	J/mol×K	903.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348906&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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