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

Inchi: InChI=1S/C17H28O4/c1-4-5-6-7-8-9-10-13-20-16(18)11-12-17(19)21-14-15(2)3/h8-9,11-
InchiKey: BDDBPKMOUGINEJ-UONSLQGUSA-N
Formula: C17H28O4
SMILES: CCCCCC=CCCOC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-217.58	kJ/mol	Joback Method
hf	-654.65	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.812		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	748.82	K	Joback Method
tc	936.23	K	Joback Method
tf	400.51	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.81	J/mol×K	748.82	Joback Method
cpg	759.96	J/mol×K	780.05	Joback Method
cpg	775.24	J/mol×K	811.29	Joback Method
cpg	789.68	J/mol×K	842.52	Joback Method
cpg	803.31	J/mol×K	873.76	Joback Method
cpg	816.17	J/mol×K	904.99	Joback Method
cpg	828.28	J/mol×K	936.23	Joback Method
dvisc	0.0011986	Pa×s	400.51	Joback Method

dvisc	0.0005206	Pa×s	458.56	Joback Method
dvisc	0.0002728	Pa×s	516.61	Joback Method
dvisc	0.0001628	Pa×s	574.66	Joback Method
dvisc	0.0001069	Pa×s	632.72	Joback Method
dvisc	0.0000753	Pa×s	690.77	Joback Method
dvisc	0.0000560	Pa×s	748.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348878&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