

Fumaric acid, isobutyl tetradec-3-enyl ester

Inchi:	InChI=1S/C22H38O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-25-21(23)16-17-22(24)26-19
InchiKey:	OFOLZDLMDLHYKI-VLDVYECUSA-N
Formula:	C22H38O4
SMILES:	CCCCCCCCC=CCCOC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]:	366.53

Physical Properties

Property code	Value	Unit	Source
gf	-175.48	kJ/mol	Joback Method
hf	-757.85	kJ/mol	Joback Method
hfus	55.19	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.762		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	2548.00		NIST Webbook
tb	863.22	K	Joback Method
tc	1058.48	K	Joback Method
tf	456.86	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.88	J/molxK	863.22	Joback Method
cpg	1057.91	J/molxK	895.76	Joback Method
cpg	1074.88	J/molxK	928.31	Joback Method
cpg	1090.83	J/molxK	960.85	Joback Method
cpg	1105.82	J/molxK	993.40	Joback Method
cpg	1119.87	J/molxK	1025.94	Joback Method
cpg	1133.05	J/molxK	1058.48	Joback Method
dvisc	0.0006816	Paxs	456.86	Joback Method
dvisc	0.0002831	Paxs	524.59	Joback Method

dvisc	0.0001438	Paxs	592.31	Joback Method
dvisc	0.0000839	Paxs	660.04	Joback Method
dvisc	0.0000541	Paxs	727.77	Joback Method
dvisc	0.0000376	Paxs	795.49	Joback Method
dvisc	0.0000277	Paxs	863.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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