

Fumaric acid, dec-4-enyl hexyl ester

Inchi:	InChI=1S/C20H34O4/c1-3-5-7-9-10-11-12-14-18-24-20(22)16-15-19(21)23-17-13-8-6-4-2
InchiKey:	BQKRFBQMBYIGSE-QLJIQFCGSA-N
Formula:	C20H34O4
SMILES:	CCCCCC=CCCCOC(=O)C=CC(=O)OCCCCC
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-189.88	kJ/mol	Joback Method
hf	-711.29	kJ/mol	Joback Method
hfus	53.53	kJ/mol	Joback Method
hvap	78.34	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.126		Crippen Method
mvol	298.940	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook
tb	817.90	K	Joback Method
tc	1006.76	K	Joback Method
tf	449.32	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.35	J/molxK	817.90	Joback Method
cpg	994.93	J/molxK	975.28	Joback Method
cpg	981.37	J/molxK	943.80	Joback Method
cpg	966.96	J/molxK	912.33	Joback Method
cpg	951.68	J/molxK	880.85	Joback Method
cpg	935.49	J/molxK	849.38	Joback Method
cpg	1007.70	J/molxK	1006.76	Joback Method
dvisc	0.0000403	Paxs	817.90	Joback Method

dvisc	0.0000537	Paxs	756.47	Joback Method
dvisc	0.0000752	Paxs	695.04	Joback Method
dvisc	0.0001123	Paxs	633.61	Joback Method
dvisc	0.0001831	Paxs	572.18	Joback Method
dvisc	0.0003356	Paxs	510.75	Joback Method
dvisc	0.0007261	Paxs	449.32	Joback Method

Sources

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=U348941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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