

Fumaric acid, heptyl tridecyl ester

Inchi:	InChI=1S/C24H44O4/c1-3-5-7-9-10-11-12-13-14-16-18-22-28-24(26)20-19-23(25)27-21-
InchiKey:	VMBCMCKYTBDXEI-FMQUUCBEESA-N
Formula:	C24H44O4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)OCCCCCCC
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
gf	-236.42	kJ/mol	Joback Method
hf	-911.07	kJ/mol	Joback Method
hfus	63.69	kJ/mol	Joback Method
hvap	87.29	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.910		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	876.36	kPa	Joback Method
rinsol	2777.00		NIST Webbook
tb	905.26	K	Joback Method
tc	1108.91	K	Joback Method
tf	499.48	K	Joback Method
vc	1.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.55	J/molxK	905.26	Joback Method
cpg	1210.11	J/molxK	939.20	Joback Method
cpg	1228.39	J/molxK	973.14	Joback Method
cpg	1245.42	J/molxK	1007.08	Joback Method
cpg	1261.26	J/molxK	1041.03	Joback Method
cpg	1275.94	J/molxK	1074.97	Joback Method
cpg	1289.52	J/molxK	1108.91	Joback Method
dvisc	0.0004895	Paxs	499.48	Joback Method
dvisc	0.0002235	Paxs	567.11	Joback Method

dvisc	0.0001206	Paxs	634.74	Joback Method
dvisc	0.0000733	Paxs	702.37	Joback Method
dvisc	0.0000486	Paxs	770.00	Joback Method
dvisc	0.0000345	Paxs	837.63	Joback Method
dvisc	0.0000257	Paxs	905.26	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348808&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

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