

Fumaric acid, 2-methylpentyl tridecyl ester

Inchi:	InChI=1S/C23H42O4/c1-4-6-7-8-9-10-11-12-13-14-15-19-26-22(24)17-18-23(25)27-20-2
InchiKey:	NUGFTGNLNMBQAA-ISLYRVAYSA-N
Formula:	C23H42O4
SMILES:	CCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)CCC
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-247.28	kJ/mol	Joback Method
hf	-895.71	kJ/mol	Joback Method
hfus	57.58	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.376		Crippen Method
mvol	345.510	ml/mol	McGowan Method
pc	932.92	kPa	Joback Method
rinpol	2572.00		NIST Webbook
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tb	881.94	K	Joback Method
tc	1079.77	K	Joback Method
tf	473.21	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.31	J/molxK	881.94	Joback Method
cpg	1211.70	J/molxK	1046.80	Joback Method
cpg	1197.28	J/molxK	1013.83	Joback Method
cpg	1181.78	J/molxK	980.86	Joback Method
cpg	1165.14	J/molxK	947.88	Joback Method
cpg	1147.33	J/molxK	914.91	Joback Method
cpg	1225.06	J/molxK	1079.77	Joback Method
dvisc	0.0000273	Paxs	881.94	Joback Method

dvisc	0.0000371	Paxs	813.82	Joback Method
dvisc	0.0000533	Paxs	745.70	Joback Method
dvisc	0.0000824	Paxs	677.58	Joback Method
dvisc	0.0001403	Paxs	609.45	Joback Method
dvisc	0.0002732	Paxs	541.33	Joback Method
dvisc	0.0006444	Paxs	473.21	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=U348731&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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