

Fumaric acid, 4-octyl hept-2-yl ester

Inchi: InChI=1S/C19H34O4/c1-5-8-10-12-16(4)22-18(20)14-15-19(21)23-17(11-7-3)13-9-6-2/h1-19
InchiKey: WYDVFLIZPNRWNR-CCEZHUSRSA-N
Formula: C19H34O4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)OC(CCC)CCCC
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-283.40	kJ/mol	Joback Method
hf	-818.43	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.957		Crippen Method
mvol	289.150	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	2066.00		NIST Webbook
rinpol	2066.00		NIST Webbook
tb	789.98	K	Joback Method
tc	976.37	K	Joback Method
tf	413.13	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.08	J/molxK	789.98	Joback Method
cpg	902.61	J/molxK	821.05	Joback Method
cpg	919.15	J/molxK	852.11	Joback Method
cpg	934.72	J/molxK	883.18	Joback Method
cpg	949.36	J/molxK	914.24	Joback Method
cpg	963.08	J/molxK	945.31	Joback Method
cpg	975.91	J/molxK	976.37	Joback Method
dvisc	0.0012655	Paxs	413.13	Joback Method

dvisc	0.0005031	Paxs	475.94	Joback Method
dvisc	0.0002480	Paxs	538.75	Joback Method
dvisc	0.0001417	Paxs	601.56	Joback Method
dvisc	0.0000900	Paxs	664.36	Joback Method
dvisc	0.0000618	Paxs	727.17	Joback Method
dvisc	0.0000451	Paxs	789.98	Joback Method

Sources

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=U405622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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